

Process Simulation Essentials

Example Book

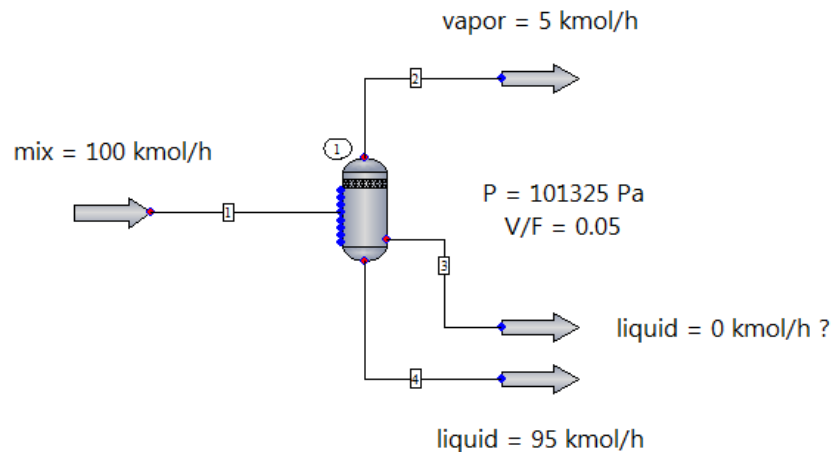


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Thermodynamics Selection: Chemicals



The selection of K-value and enthalpy models is the most critical step in process simulation. An improper selection leads to unreliable results.

Once you have selected all the components involved in the process, the Thermodynamics Wizard dialog box will appear. You can either click **Cancel** to enter thermodynamics manually, or enter parameters. In this example, an equimolar mixture of acetonitrile and benzene is flashed with specified $P = 101325$ and vapor fraction = 0.05.

With this example, you can learn about the typical K-value models used for non-ideal solutions. These K-value models are based upon the excess Gibbs free energy and use activity coefficient methods (e.g. Wilson, NRTL, UNIQUAC, and UNIFAC), as well as binary interaction parameters (BIPs).

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics called "Types of Solutions" and "Thermodynamics."

Using the Thermodynamics Wizard (using default conditions):

Select **Thermophysical > Thermodynamics Wizard**, then click **OK**. Considering the components and the T and P range, the wizard selects NRTL as the K-value and Latent Heat as the enthalpy model. The next step is the Thermodynamic Settings dialog, where you can make further changes or override the selection made by the wizard. Click **OK** to accept the selection. The window containing the NRTL binary interaction parameters (BIPs) appears next.

Note: Use the wizard tool as a starting point. Proper selection of thermodynamics is the engineer's responsibility. Your simulation may call for the use of a different model than what the wizard suggests.

For instance, the acetonitrile/nitromethane system is fairly ideal, and using the Ideal Vapor Pressure (Raoult's Law) or an activity coefficient model (NRTL, UNIQUAC) won't make much difference. This is not the case for acetonitrile/benzene or benzene/water, where the departure from ideal behavior is strong. For instance, the acetonitrile/benzene forms an azeotrope, and the benzene/water system exhibits liquid-liquid and vapor-liquid-liquid equilibrium.

Entering thermodynamics manually:

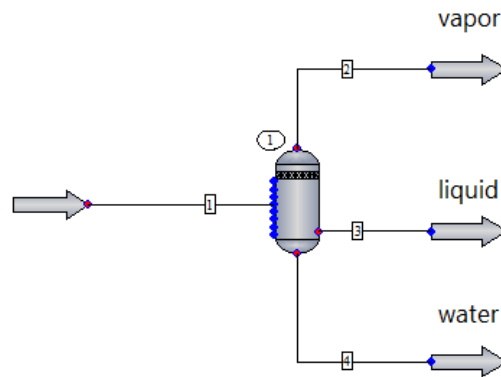
Suppose you want to use UNIQUAC or UNIFAQ instead of NRTL. Go to **Thermophysical > Thermodynamic Settings** and change the K-value model for UNIQUAC, but leave the enthalpy Model as it is (Latent Heat). Does choosing UNIQUAC give a different result for the flash calculation? What about when you choose UNIFAQ?

Note: In the K-value Models tab, change the Global Phase Option to Vapor/Liquid/Liquid/Solid so that if liquid-liquid equilibrium exists, stream 3 will contain the light liquid phase.

To use this example, select a pair of components and specify composition in the feed. Choose the K-value (**Thermodynamics > Thermodynamic Settings > Global K-value Model**). Run the simulation and evaluate the results for the liquid streams. Notice any differences among Ideal Vapor Pressure (VAP), NRTL, UNIQUAC, and UNIFAC. Notice if more than one liquid phase exists. Select Stream 1, then go to **Plot > TPXY** and select the pair of components, fix the pressure, and click **OK** to generate a TXY diagram and XY diagram.

To learn more about selection of thermodynamic methods, visit www.chemstations.com/Support/ and download the PDF "Selection of Thermodynamic Methods" under Top Articles. See Appendix III, "Thermodynamic Model Selection—Application Tables."

Thermodynamics Selection: Hydrocarbons



The selection of K-value and enthalpy models is the most critical step in process simulation. An improper selection leads to unreliable results.

Once you have selected all the components involved in the process, the Thermodynamics Wizard dialog box appears. You can either click **Cancel** to enter thermodynamics manually, or enter the desired parameters. In this example, a mixture of hydrocarbons and water is flashed at $T = 300$ K and $P = 690$ kPa.

Using the wizard (using default conditions): **Thermophysical** > **Thermodynamics Wizard**, then click **OK**.

Using the wizard (specifying process conditions): **Thermophysical** > **Thermodynamics Wizard** and enter the temperature (260-360 K) and pressure range (101325-700000 Pa) for the process, then click **OK**.

Considering the components and the T and P range, the wizard selects Soave-Redlich-Kwong (SRK) as both the K-value and enthalpy models. The next step is the Thermodynamic Settings dialog box, where you can make further changes or override the selection made by the wizard. Notice that the Water/Hydrocarbon Solubility is marked as Immiscible. As a result, Stream 4 has pure water.

Note: If water is not part of the process but is used as a utility, it is recommended that you select water as a component to ignore in the wizard dialog box, to prevent a misleading selection.

Importance of T and P range: Suppose the process occurs at very low temperature (< -70 °C) and high pressure (> 10000000 Pa). Go to the wizard and enter a T range of 180 to 250 K and a P range of 101325 to $1e+06$ Pa.

Notice how the temperature and pressure range affects the selection. CHEMCAD now selects Peng-Robinson (PR) instead. PR is a common selection when the process conditions are extreme.

Note: Use the wizard as a starting point. Proper selection of thermodynamics is the engineer's responsibility. Your simulation may call for the use of a different model than what the wizard suggests.

Entering thermodynamics manually: Suppose you want to use Peng-Robinson (PR) instead of SRK, even if the process conditions are not extreme. Go to **Thermophysical** > **Thermodynamic**

Settings and change the K-value model for PR, then click on the Enthalpy Models tab and select PR as well. Does choosing PR give a different result for the flash calculation?

To learn more about selection of thermodynamic methods, visit www.chemstations.com/Support/ and download the PDF "Selection of Thermodynamic Methods" under Top Articles. See Appendix III, "Thermodynamic Model Selection—Application Tables."

Global and Local Thermodynamics



In this example, Flash UnitOp #1 uses global flowsheet thermodynamics (K-value = NRTL), while Flash UnitOp #2 uses local thermodynamics (K-value = UNIQUAC).

A mixture of ethanol and water at 170 °F and atmospheric pressure is used for this example. Both Flash UnitOps have the same specifications.

To review or change the Global K-value: **Thermophysical** > **Thermodynamic Settings** > **K-value Models** tab > **Global K-value Model** and select from the drop-down menu.

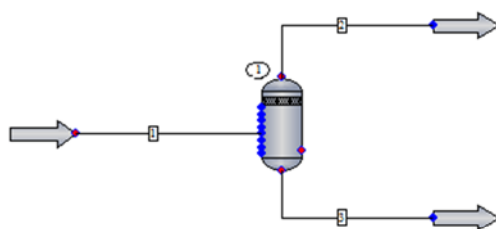
To set local thermodynamics: **Thermophysical** > **Thermodynamic Settings** > **K-value Models** tab and check the **Set local thermodynamics** option. Enter **2** for the the UnitOp ID and click **OK**. A new dialog box will appear, where you can select a different K-value (and/or enthalpy model) for the UnitOp.

To review the thermodynamics for the flowsheet, select **Report** > **Thermodynamics**. Notice that the vapor fraction and enthalpy of the feed are governed by the Global K-value. Then, the Flash UnitOp flashes the feed using the local K-value, thus giving a slightly different result.

This feature is often used when the phase equilibrium calculations for a unit within the process require a particular Equation of State or Activity Coefficient model.

To see this in action, go to the **My Simulations\Examples-7.xx\Biodiesel** folder and open the example simulation called "Acid-catalyzed biodiesel." Another good example to try is "Post-combustion CC - MEA" under the **Carbon Capture** folder.

Binary Interaction Parameter (BIP) Regression



BIPs	CHEMCAD BIPs	DECHEMA BIPs	Regressed BIPs
B _{ij}	377.58	317.55	354.41
B _{ji}	653.89	602.56	608.40
Alpha _{ij}	0.586	0.534	0.526

This example details how to review available BIPs in CHEMCAD's database, enter BIPs manually, and regress BIPs from VLE data. This is an advanced topic.

Binary Interaction Parameters (BIPs) are empirical interaction parameters specific to an i-j molecular pair.

To learn more about BIPs, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Overview of BIPs in CHEMCAD."

First, three BIP sets were created by selecting **Thermophysical > Thermodynamic Settings > K-value Models** tab and entering **3** under **No. of BIP sets**.

Set 1 uses built-in BIPs from CHEMCAD's database. Go to **Thermophysical > Component Database > Database BIPs** and choose any pair of components to review available BIPs.

Set 2 has BIP parameters entered manually. Go to **Thermophysical > Edit BIPs**. Here, the recommended values found in DECHEMA's Chemistry Data Series - Vapor-Liquid Equilibrium Data Collection for the Acetone/Water binary system were entered in the B_{ij}, B_{ji}, and Alpha_{ij} columns, thus overriding CHEMCAD's built-in parameters.

Note: the values as shown on the reference have been divided by Gas constant R in CHEMCAD R = 1.98721 cal/mol/deg.K to make them comparable to CHEMCAD's.

Set 3 was created after regressing VLE data for acetone (1)/water (2) at a constant pressure of 1.013 bar from the same source. To perform a BIP regression, select **Thermophysical > Regress BIPs**. Select the components, then **Regress TPxy/Pxy/Txy VLE data** and enter data in the appropriate columns. (For more, see the "BIP Regression" help topic.)

Note: The first component you select will be treated as the i component by the program. Make sure that your selection matches the proper i component in the VLE data.

Review the flowsheet specifications and BIPs by selecting **Report > Thermodynamics**.

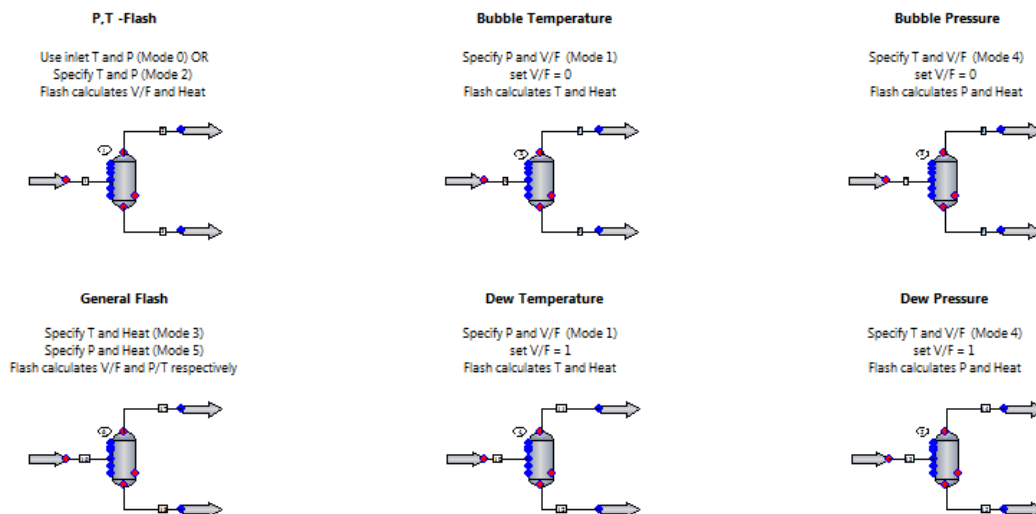
Note: i and j refer to the order in the component list (i.e., acetone = 1; water = 2).

To compare the results, activate the BIP set first: **Thermophysical > Thermodynamic settings > K-value models > Default BIP set**. Type the number of the BIP set of interest, and then run the simulation. Do results differ when using the various BIP sets?

Reference:

Gmehling et al. "Vapor-Liquid Equilibrium Data Collection", Chemistry Data Series, vol. I, part 1b, DECHEMA, Frankfurt/Main, 1988. pp. 146 and 153.

Flash Calculations



In Vapor-Liquid Equilibrium (VLE), liquid and vapor phases coexist in equilibrium. When the overall composition is known (feed composition), then two variables are required to fix the state of the system.

The Flash UnitOp modes offer combinations of variables to be specified: temperature, pressure, vapor fraction, and duty.

Based on the feed composition and conditions, the Flash UnitOp calculates the other variables, as well as the quantities and compositions of the vapor and liquid phases in equilibrium.

Modes 0 and 2: Use inlet T and P or Specify T and P, respectively.

Modes 1 and 4: Specify vapor fraction (V/F) and P or T, respectively.

Modes 3 and 5: Specify T or P and heat duty (H), respectively.

Modes 6 and 7: Specify P or T and perform isentropic flash, respectively (not shown in this example).

Modes 8 and 9: Specify P or T and water dew point T or P, respectively (not shown in this example).

This example shows the typical Flash calculations using an equimolar mixture of benzene (1)/ethylbenzene (2), which is wide-boiling and thus easily separated.

Additional exercises:

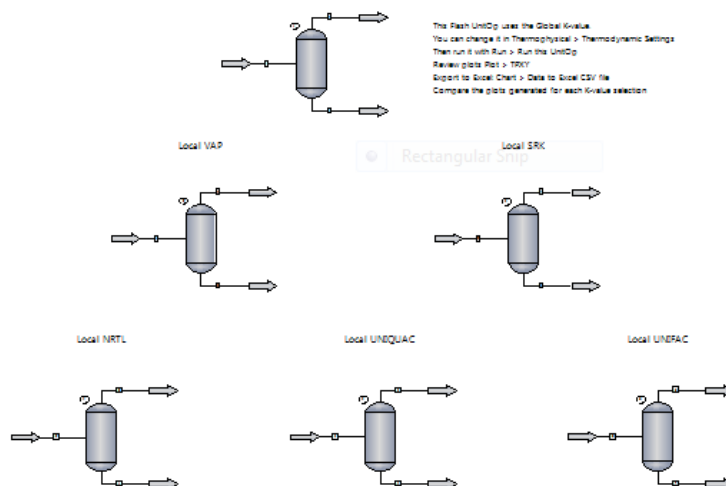
- Change feed conditions and observe how calculations change.
- Nonequimolar mixture of benzene (1)/ethylbenzene (2).
- Benzene (1)/toluene (2) mixture at various compositions.
- Benzene (1)/cyclohexane (2) mixture at various compositions. Can you find the azeotropic composition?
- Benzene (1)/toluene (2)/ethylbenzene (3) mixture.

To generate binary TPXY plots, select the feed stream, go to **Plot > TPXY**, and select the two components (1 for the most volatile) and either constant pressure (PXY) or constant temperature (TXY).

Reference:

Smith J.M., Van Ness, H.C. & Abbott M.M. "Introduction to Chemical Engineering Thermodynamics." Seventh Edition, McGraw-Hill. pp. 341-347, 367-369.

Vapor-liquid Equilibrium: Non-ideal Systems



In this example, the Flash UnitOp is used to model a single vapor-liquid equilibrium stage.

All Flash UnitOps have Mode 2 specified (**Specify T and P; calculate V/F and Heat**). You can specify other modes to perform various calculations. See the example called **_Process Simulation Essentials\2 Phase Equilibria\1 - Flash calculations**.

With this example, you can learn about the typical K-value models used for non-ideal solutions. These K-value models are based upon the excess Gibbs free energy and use activity coefficient methods (e.g., Wilson, NRTL, UNIQUAC, and UNIFAC), as well as Binary Interaction Parameters (BIPs).

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Types of Solutions" and "Thermodynamics."

CHEMCAD has built-in BIPs from numerous chemical components in the database. Select **Thermophysical > Component Database > Database BIPs** and choose any pair of components to review available BIPs.

Notice how the K-value selection determines the molar rate and composition for the vapor and liquid products once the flash calculation is performed.

Select **Format > Add Stream Box > Product Streams** to generate a table to compare the K-value models side by side.

You can test for two different systems as specified below. This example has case a) set up and NRTL as the global K-value.

a) Positive deviation from Raoult's Law: Methyl Ethyl Ketone (1)/Toluene (2) at $T = 50\text{ }^{\circ}\text{C}$ and $P = 20\text{ kPa}$

b) Negative deviation from Raoult's Law: Tetrahydrofuran (1)/Carbon Tetrachloride (2) at $T = 30\text{ }^{\circ}\text{C}$ and $P = 20\text{ kPa}$ (change the specification for the Flash UnitOp too)

Local K-values have been used for the Flash UnitOps. The first Flash UnitOp (1) has Global K-value, which can be modified by selecting **Thermophysical > Thermodynamic Settings > Global K-value Model**.

Note: Plots are generated using the Global K-value. Match the Global K-value to any of the K-value models in the flowsheet. Then run the top Flash UnitOp (1). Select Stream 1 and go to **Plot > TPXY**.

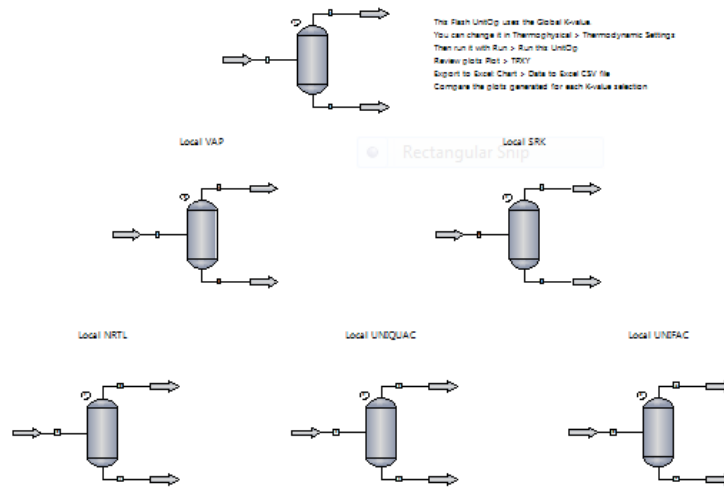
Note: The use of local thermodynamics is for illustrative purposes as it is not typical to have that many local K-value models in a single flowsheet.

Review the flowsheet specifications and BIPs for each activity coefficient by selecting **Report > Thermodynamics**. Note that I and J refer to the order in the component list.

Reference:

Smith J.M., Van Ness, H.C. & Abbott M.M. "Introduction to Chemical Engineering Thermodynamics." Seventh Edition, McGraw-Hill. pp. 348-350, 352-356, 435-439.

Vapor-liquid Equilibrium: Azeotropes



In this example, the Flash UnitOp is used to model a single vapor-liquid equilibrium stage.

All Flash UnitOps have Mode 1 specified (**Specify V/F and P; calculate T and Heat**). You can specify other modes to perform various calculations. See the example called **_Process Simulation Essentials\2 Phase Equilibria\1 - Flash calculations**.

With this example, you can learn about the typical K-value models used for non-ideal solutions. These K-value models are based upon the excess Gibbs free energy and use activity coefficient methods (e.g., NRTL, UNIQUAC, and UNIFAC), as well as Binary Interaction Parameters (BIPs).

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Types of Solutions" and "Thermodynamics."

Activity coefficient methods are used in processes where the solution is non-ideal or highly non-ideal, two liquid phases may exist, and azeotrope(s) may exist.

CHEMCAD has built-in BIPs from numerous chemical components in the database. Select **Thermophysical > Component Database > Database BIPs** and choose any pair of components to review available BIPs.

The purpose of this example is to determine whether the mixture forms an azeotrope, and if so, at what temperature and composition this occurs.

Azeotropic mixtures are liquid mixtures that exhibit sufficiently large deviations from Raoult's Law behavior. As a result, the T-x and T-y curves exhibit a minimum (positive deviations) or a maximum (negative deviations) at constant pressure. At the azeotropic point $x_1 = y_1$ and the dewpoint and bubblepoint curves intersect. A boiling liquid of this composition (azeotropic point) produces a vapor of the same composition. No separation is possible by distillation since the solution is constant-boiling.

Notice how the K-value selection determines the azeotropic temperature and composition. Notice that the Ideal Vapor Pressure and SRK models fail to detect azeotropes.

This simulation enables you to do the following:

- 1) Test whether a pair of chemical components exhibits an azeotrope at $P = 1$ bar (or other pressures).
- 2) Test whether or not a K-value method can predict the existence of such an azeotrope.
- 3) Estimate the azeotropic temperature and azeotropic point by looking at the TXY diagram (**Plot > TPXY**) and specifying pressure at 1 bar.
- 4) Estimate the azeotropic pressure and azeotropic point by looking at the PXY diagram (**Plot > TPXY**) and specifying the temperature in Celsius.
- 5) Perform flash calculations to determine dew point and bubble point of mixtures. At the azeotropic composition, bubble $T =$ dew T (for constant P).

Is the azeotropic temperature and composition the same for all K-values?

Is the azeotropic temperature and composition the same when you change the pressure?

Which of the K-values does not predict the existence of the azeotrope (when there is one)?

Possible test cases:

Ethanol (1)/water (2); ethanol (1)/benzene (2); ethanol (1)/cyclohexane (2); ethanol (1)/toluene (2); benzene (1)/cyclohexane (2); benzene (1)/toluene (2).

Note: Water exhibits Vapor-Liquid-Liquid and Liquid-Liquid equilibrium with benzene, cyclohexane, and toluene. This example DOES NOT support this calculation. Please see the example on VLLE and LLE (**_Process Simulation Essentials\2 Phase Equilibria\4 - VLLE and LLE**) instead.

This example shows the ethanol (1)/water (2) system at constant $P = 1$ bar. The composition of the feed is close to the azeotropic point.

Local K-values have been used for the Flash UnitOps. The first Flash UnitOp (1) has a global K-value, which can be modified in **Thermophysical > Thermodynamic Settings > Global K-value Model**.

Note: Plots are generated using the global K-value. Match the global K-value to any of the K-value models in the flowsheet. Then run the top Flash UnitOp (1). Select Stream 1 and go to **Plot > TPXY**.

Note: The use of local thermodynamics here is for illustrative purposes, as it is not typical to have that many local K-value models in a single flowsheet.

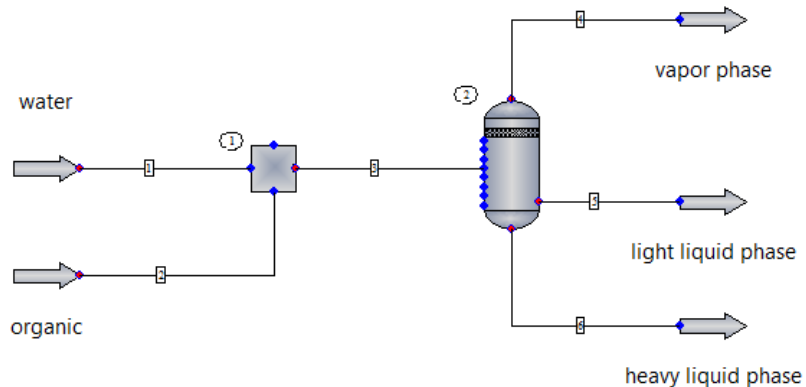
Review the flowsheet specifications and BIPs for each activity coefficient under **Report > Thermodynamics**.

Note: I and J refer to the order in the component list.

Reference:

Smith J.M., Van Ness, H.C. & Abbott M.M. "Introduction to Chemical Engineering Thermodynamics." Seventh Edition, McGraw-Hill. pp. 347-355, 446-449, 474-475.

Vapor-liquid-liquid and Liquid-liquid Equilibrium



In this example, water is mixed with an organic feed and flashed at the inlet temperature and pressure conditions.

NRTL was selected as the K-value for this example because it can predict liquid-liquid equilibrium.

Note: The Global Phase Option has been changed to Vapor/Liquid/Liquid/Solid to allow this calculation. This is set by selecting **Thermophysical > Thermodynamic Settings > K-value Models > Global Phase Option**.

To plot a TXY or PXY diagram, select stream 3, then go to **Plot > TPXY** and select the pair of components, fix the pressure (or temperature), and click **OK** to generate a TXY diagram and XY diagram.

What if you choose cyclohexane or toluene as the organic feed?

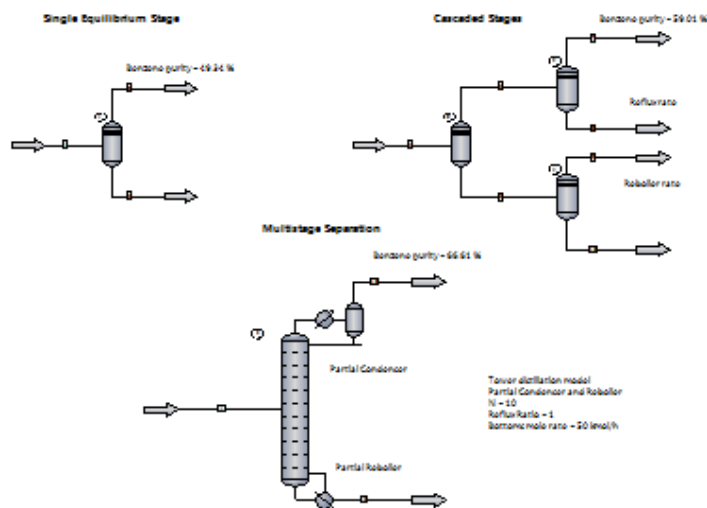
What if you change the temperature of the organic feed to 170 °F? Is there a vapor phase?

What if you exchange the water for ethanol?

What if you add ethanol to the water feed? Does ethanol split into the liquid phases?

What is the phase distribution and composition if UNIQUAC or UNIFAC is used? To find out, select **Thermophysical > Thermodynamic Settings > K-value Models > Global K-value Model > UNIQUAC**.

Distillation Basics: Benzene/Toluene



In this example, a mixture of benzene and toluene is separated according to the components' relative volatilities. With this example, you can learn the basics of multistage separation, as well as how to specify a simple Tower distillation model.

For an equilibrium stage at a given pressure, the range of possible product compositions is bound by the bubble point and dew point compositions at that pressure.

This concept is better understood by looking at the TXY diagram. Go to **Plot > TPXY** and select the components in order of relative volatility (benzene = 1, toluene = 2) at constant pressure of 1.72 bar. CHEMCAD generates TXY and XY charts.

Starting at 0.4 mole fraction of benzene (the feed composition), intersect the bubble point (bottom curve) and dew point (top curve) at $T = 118\text{ }^{\circ}\text{C}$. These are the mole fractions of benzene in the liquid and vapor products, respectively. These in turn become the feed compositions for streams 5 and 6. For stream 5, find the intersection with $T = 115\text{ }^{\circ}\text{C}$ to find the compositions of streams 7 and 8. Notice how the mole fraction of benzene in the vapor increases continuously. The same can be done for stream 6 by finding the intersection of the curves with $T = 120.5\text{ }^{\circ}\text{C}$.

Notice how the mole fraction of benzene in the liquid product decreases continuously. As more equilibrium stages are added, benzene concentrates in the vapor, while toluene concentrates in the liquid.

A distillation column consists of multiple equilibrium stages stacked together, which allows the temperature variation from state to stage in order to carry out the progressive separation.

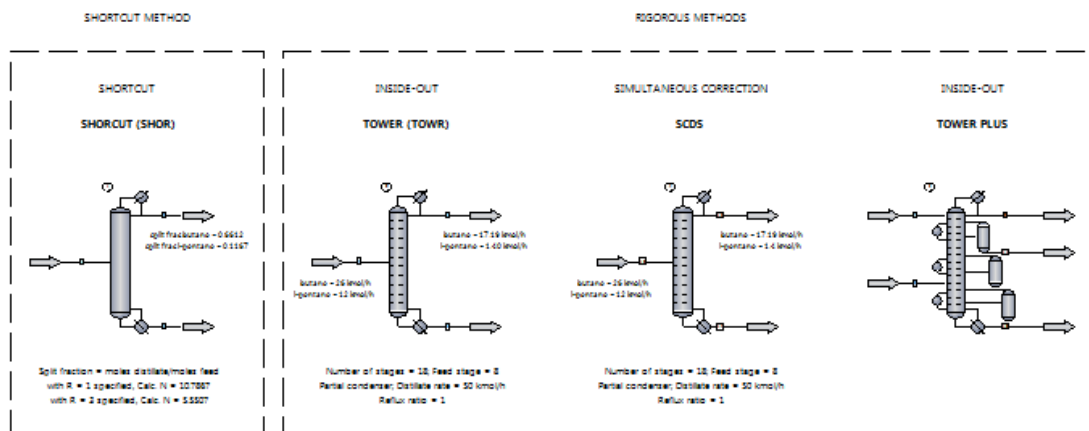
For this example, a Tower distillation column with 10 stages was used to separate the mixture. The reflux ratio was set at 1 and the bottoms mole rate at 50 kmol/h.

Determine the effect of the separation when:

1. Number of stages is increased.
2. Reflux ratio is increased (how does the calculated duty change?).
3. Bottoms rate is increased/decreased.

To learn more about column performance, see the example called **_Process Simulation Essentials\3 Separators\4 - Distillation column performance**.

Distillation Models in CHEMCAD



This example shows CHEMCAD's steady-state distillation models. A narrow-boiling hydrocarbon mixture is separated using the Tower and SCDS columns. The Shortcut column is used to get an estimate for the minimum number of stages required to split n-butane (light key) from i-pentane (heavy key).

CHEMCAD offers both shortcut and rigorous methods for solving multicomponent distillation problems. The shortcut method uses non-rigorous thermodynamics, and is based on the assumption of constant molal overflow, which does not happen in reality. Both rigorous methods use thermodynamics to calculate mass and energy balances, which model real behavior.

The Shortcut model (SHOR) uses the Fenske-Underwood-Gilliland method. Both rating and design cases are provided.

For this example, design mode was used to calculate the minimum number of stages required when reflux ratio and the split fractions of light key and heavy key components are specified.

Note: This method may not be suitable for column design and may give incorrect results in systems with azeotropes. It should be used to obtain only an estimate for the minimum number of stages before designing a Tower or SCDS column.

The Tower model (TOWR) uses the inside-out rigorous method for multistage VLE.

The SCDS model (SCDS) uses the simultaneous corrections method for multistage VLE.

For this example, both the TOWR and the SCDS models were specified in the same way. They use different mathematical algorithms and number of iterations to converge to a solution, but the solution will be the same. When computers were less powerful, the choice between TOWR and SCDS was related to the process in question. TOWR usually requires fewer iterations and converges faster, but this is not as relevant using modern computers. However, the SCDS allows for special distillation cases that TOWR does not support.

The Tower Plus model uses the inside-out rigorous method too, but allows for complex columns. For this example, the model has not been specified. This model is very difficult to converge and is used for petroleum and refining applications.

To see the Tower Plus model at work, see the example at **My Simulations\Examples-7.xx\Distillation and Absorption\Atmospheric Distillation of Crude Oil**. This example uses distillation curves to characterize the oil feed.

All three rigorous models will solve standard absorbers, strippers, and fractionators, with and without reboilers, condensers, multiple feeds, and multiple draws. The choice among models is more easily made by exception:

SHOR: 1) Constant molal overflow, non-rigorous thermodynamics.

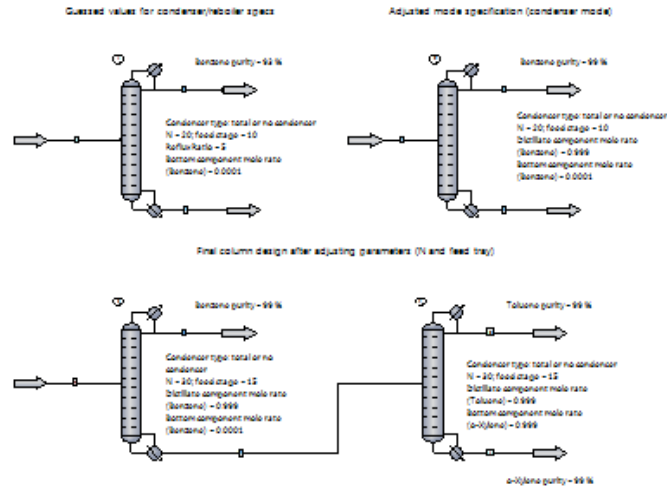
TOWR: 1) Tray condition specification.

TOWER PLUS: 1) Tray condition specification; 2) Side strippers and pumparounds.

SCDS: 1) Tray efficiency less than 100% (Murphree efficiency); 2) Mass transfer model (packed or tray column); 3) Reactive distillation; 4) Highly non-ideal thermodynamics; 5) Electrolytes.

To learn more, press **[F1]** to open the CHEMCAD help file, then search for the help topic that addresses the particular distillation model.

Column Design: Benzene/Toluene/Xylene



In this example, a mixture of benzene, toluene, and o-xylene is separated to produce three product streams each at least 99.9 mole % pure.

The first step is to design a column that separates mostly benzene in the overhead. This requires guessing or estimating the column stages, feed tray location, and mode specification.

For this example, a Tower distillation column with 10 stages, total condenser, and reboiler was used to separate the mixture. The feed enters at tray 10. A reflux ratio of 5 was set as the condenser mode specification, and a mole fraction of 0.0001 of benzene in the bottom was set as the reboiler mode specification.

With these specifications, the overhead purity does not reach the 99.9 mole % target. By specifying component mole fraction of benzene (=0.999) instead of reflux ratio, we allow the reflux ratio to vary until the mass balance is achieved. The calculated reflux ratio turns out to be 19.16.

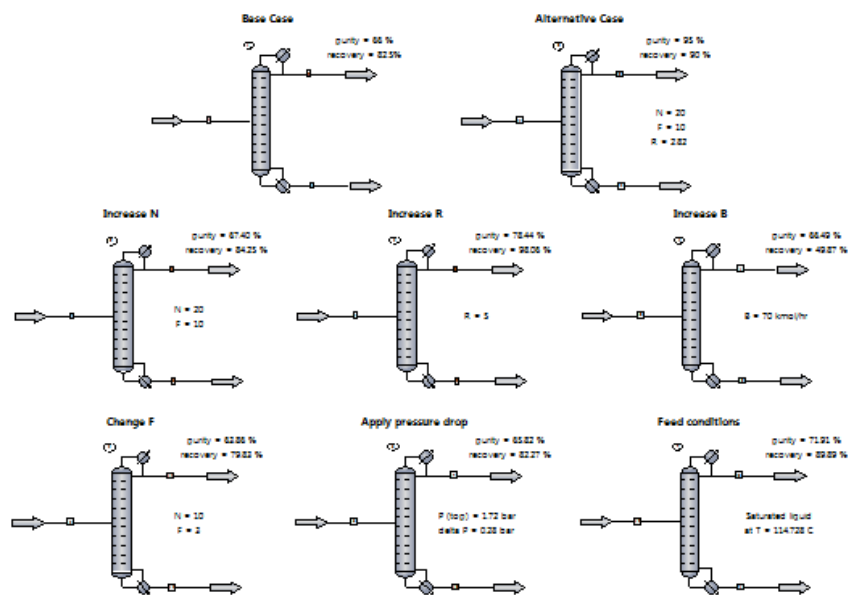
This reflux ratio is quite large. It can be decreased by increasing the number of stages (e.g., 30 stages) and/or relocating the feed tray. Specifying $N = 30$ and feed tray = 15 gives a reflux ratio of 2.3.

Once the benzene has been separated, a second column is needed to separate toluene from o-xylene. The procedure is the same as for the first column. The condenser mode specification is set at 0.999 mole fraction of toluene in the distillate, while the reboiler mode specification is set at 0.999 mole fraction of o-xylene. Using 20 stages and feeding the bottoms of the first column to the second column at tray 10 results in the desired separation, with a reflux ratio of 5.4 for UnitOp 4. Specifying $N = 30$ and feed tray = 15 lowers the reflux ratio to 1.8, and gives 99.9 mole % products.

To obtain a summary of results for the column(s), select **Report > UnitOps > Select UnitOps**. For tabulated results, right-click the UnitOp and select **View Column Profile**. Select **Plot Column Profile** from the right-click menu to generate plots for the temperature profile, total vapor flow, and/or total liquid flow.

Note: In the Tower dialog box, under the Convergence tab, notice that the mode 6 (**Auto Estimation**) is used. This means that CHEMCAD will try its best to make the column converge. In the case that the mode specifications are unfeasible, the UnitOp ID will turn yellow and CHEMCAD will issue a warning: "Can't converge with original specs. Alternative optimal solution is found."

Column Performance: Benzene/Toluene



In this example, a mixture of benzene and toluene is separated to produce a distillate product containing at least 95 mole % benzene. The alternative design should maximize benzene recovery (i.e., mole rate of benzene in the distillate over benzene mole rate in the feed) and use a reasonable number of stages and reflux ratio.

The base case column is designed as follows:

Condenser type: total or no condenser
 Number of stages (N) = 10
 Feed stage (F) = halfway
 50 % vaporized feed
 Pressure = 1.72 bar (constant)
 Reflux Ratio (R) = 1
 Bottoms mole rate (B) = 50 kmol/h

Then, the effect of changing a parameter or specification is investigated. This activity can be carried out automatically using the Sensitivity Study feature. To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Sensitivity Study." You can also see the example called **_Process Simulation Essentials\9 Tools\3 - Sensitivity study - distillation**.

As a sample, a sensitivity study named "FeedLoc" has been conducted. It records the mole fraction of benzene in the distillate as the feed location is changed from N = 2 to N = 9 in equal steps.

To load the sensitivity study, select **Run > Sensitivity Study > FeedLoc > Run All**, then click **Yes** to reset to the original state.

To review the input for the study, select **Run > Sensitivity Study > FeedLoc > Edit**.

To review the results, select **Run > Sensitivity Study > FedLoc > Report Results**. This report indicates the optimum feed location to be tray 5.

Note: The sensitivity study enables you to test multiple cases efficiently, but it does not provide you the optimum answer.

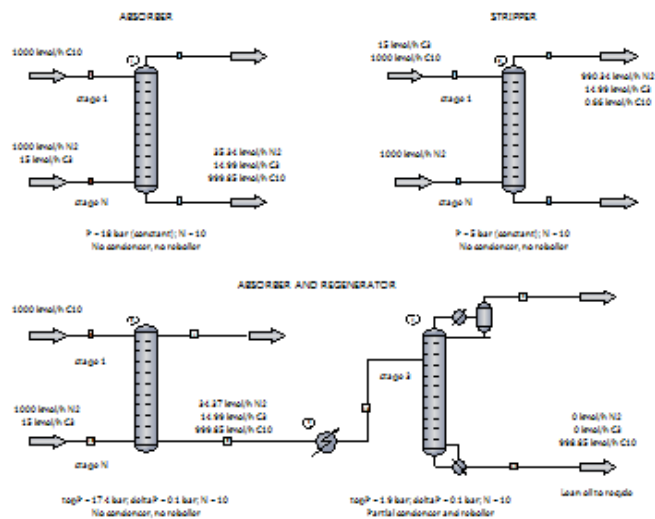
The "alternative case" achieves the specified separation while maximizing recovery and minimizing reflux ratio.

With this example, you can experiment with the specifications and compare the results to the base case. By doing this, you can identify trends and design an optimization strategy. Finding the optimum usually involves the interplay of many parameters and specifications, as well as economic considerations. Column design is often a trial-and-error process.

The alternative design achieves 95% purity and 90% recovery of benzene in the distillate. The feed conditions and pressure drop were not changed with respect to the base case. The number of stages and feed location were adjusted to maintain the reflux ratio below 3.

To obtain a summary of results for the column(s), select **Report > UnitOps > Select UnitOps**. For tabulated results, right-click the UnitOp and select **View Column Profile**. Select **Plot Column Profile** from the right-click menu to generate plots for the temperature profile, total vapor flow, and/or total liquid flow.

Absorption and Stripping



This example shows the configuration and performance of an absorption column (UnitOp 1) and a stripping column (UnitOp 2). Propane is the key component in both cases—that is, the component which is transferred from one phase to the other, with nitrogen mostly in the vapor phase and decane in the liquid phase.

Absorption column:

The absorbent (i.e., liquid) is fed at the top of the column and the mixture containing the key component is fed at the bottom. The streams flow countercurrently and propane is absorbed into the liquid phase.

Stripping (or desorption) column:

The stripping agent (i.e., gas) is fed at the bottom of the column and the mixture containing the key component is fed at the top. The streams flow countercurrently and propane is transferred to the vapor phase.

Key variables:

The component separation depends on the number of stages and the ratio of liquid-to-vapor feed rates. The identity of the absorbent or stripper also affects the performance.

What if you increase or decrease the number of stages?

Note: Streams 2 and 6 should always enter the bottom of the column, so change the feed stage to be the same as the number of stages.

What if you increase or decrease the flow rate of decane (1) or nitrogen (2)?

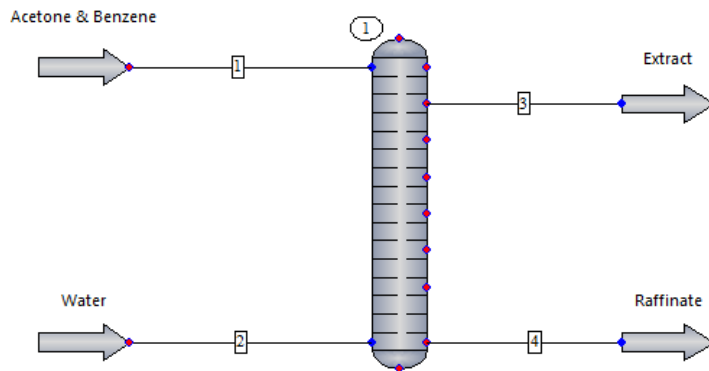
What if you use dodecane (i.e., a heavier liquid) as the absorbent instead?

Next, this example shows an absorption column followed by a desorption column (a.k.a. regenerator). First, propane is recovered by absorption using decane. Then, decane is regenerated (i.e., recovered and recycled back to the absorption column) in the desorption column. This arrangement is typical of processes involving the absorption of impurities feeding the heavy solvent at stage 1 and the regeneration of such solvent in a desorption/regeneration step. Typical processes include gas sweetening and gas dehydration.

For relevant examples, see the **My Simulations\Examples-7.xx\Gas Processing** folder.

To obtain a summary of results for the column(s), select **Report > UnitOps > Select UnitOps**. For tabulated results, right-click the UnitOp and select **View Column Profile**. Select **Plot Column Profile** from the right-click menu to generate plots for the temperature profile, total vapor flow, and/or total liquid flow.

Liquid-liquid Extraction



In this example, a countercurrent Liquid/Liquid Extractor (EXTR) with 7 stages is used to recover acetone from a mixture with benzene. The acetone and benzene enter the extractor at stage 1, while water enters at the bottom. This simulation achieves 99.96% recovery of acetone in the extract.

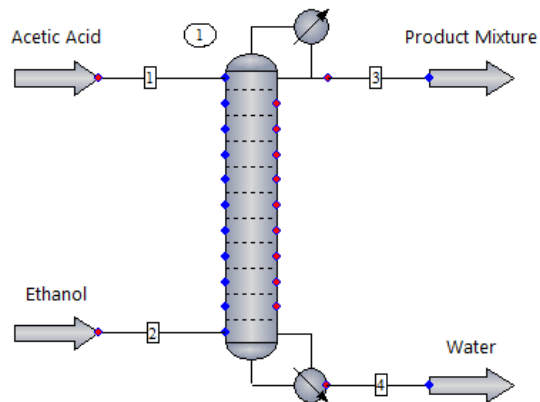
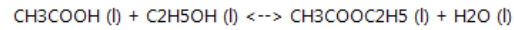
The solvent (water) and the feed are two essentially immiscible liquids. The solute (acetone), to be extracted from benzene by water, is soluble in both phases.

You can confirm this by selecting **Plot > Binary LLE** and choosing any combination of two components (acetone-benzene, acetone-water, or water-benzene).

Two key design variables are 1) number of trays and 2) water flow rate. This example shows the optimized design, but you can still modify the number of trays, feed location, and water flow rate to see the effects in the separation.

NRTL was selected as the K-value because it serves to model the non-ideal behavior in the liquid phase.

Ethyl Acetate by Reactive Distillation



This example shows a reactive distillation of an extremely non-ideal system using an SCDS distillation column. It involves an esterification reaction between ethanol and acetic acid to form ethyl acetate and water.

In reactive distillation, phase equilibrium and chemical reaction occur in the same equipment. Phase separation is controlled by phase equilibrium relations or rate-based mass and heat transfer mechanisms (i.e., packed columns); chemical reactions are controlled by chemical equilibrium relations or by reaction kinetics. The reaction takes place in the liquid phase.

Kinetic data for the forward and backward reaction were entered into the column. Double-click on the column (1) to open the SCDS Distillation Column dialog box. Notice that **Check here for reactive distillation** is checked. Click **OK** to open the Reactive Distillation Data menu, then click on the options to review the input data.

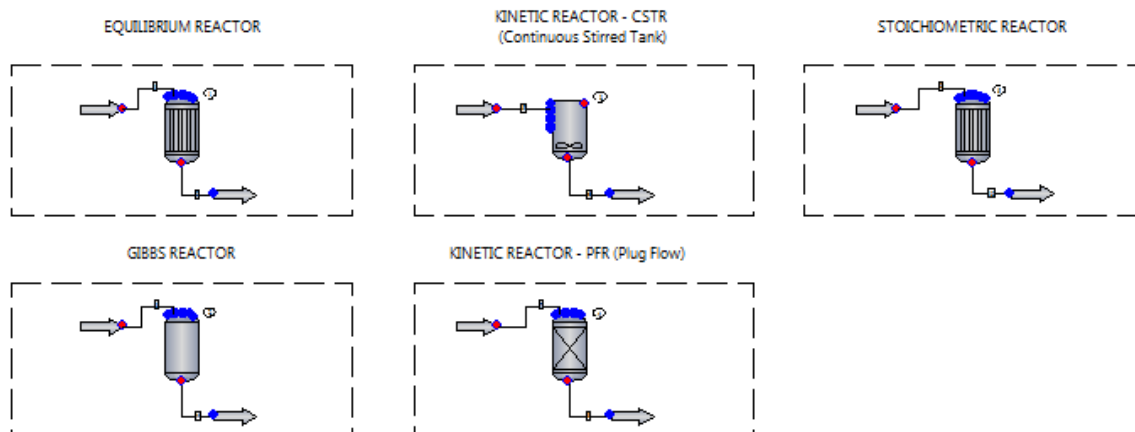
NRTL Binary Interaction Parameters (BIPs) account for this thermodynamically complex system with two liquid phases and vapor phase association.

To review BIPs, select **Report > Thermodynamics**.

To review K-value and vapor phase association selection, select **Thermophysical > Thermodynamic Settings**.

Reactor Models in CHEMCAD

Esterification Reaction: $\text{CH}_3\text{COOH} (\text{l}) + \text{C}_2\text{H}_5\text{OH} (\text{l}) \rightarrow \text{CH}_3\text{COOC}_2\text{H}_5 (\text{l}) + \text{H}_2\text{O} (\text{l})$



This example shows an esterification reaction between acetic acid and ethanol to produce ethyl acetate and water using all of CHEMCAD's reactor models, with the exception of the vessel reactor, which involves dynamics. The reaction takes place in the liquid phase and the NRTL K-value has been chosen to model the non-ideal behavior of the mixture.

For both the equilibrium reactor and the Gibbs reactor, the reaction stoichiometry for the forward reaction has been entered.

Note: The Gibbs reactor is not well suited to liquid-phase reactions. It is shown in this example to illustrate its setup.

For both the CSTR and the plug flow reactor, the reaction stoichiometry and kinetic data (frequency factor and activation energy) have been entered for both the forward and reverse reactions.

For the stoichiometric reactor, the reaction stoichiometry and fractional conversion of ethanol have been specified.

All reactor UnitOps operate isothermally at 50 °C. You may choose Adiabatic as the thermal mode when specifying the reactor.

Exercises:

What is the effect of having a higher temperature on the fractional conversion?

What is the effect of operating at a different pressure or a different pressure drop?

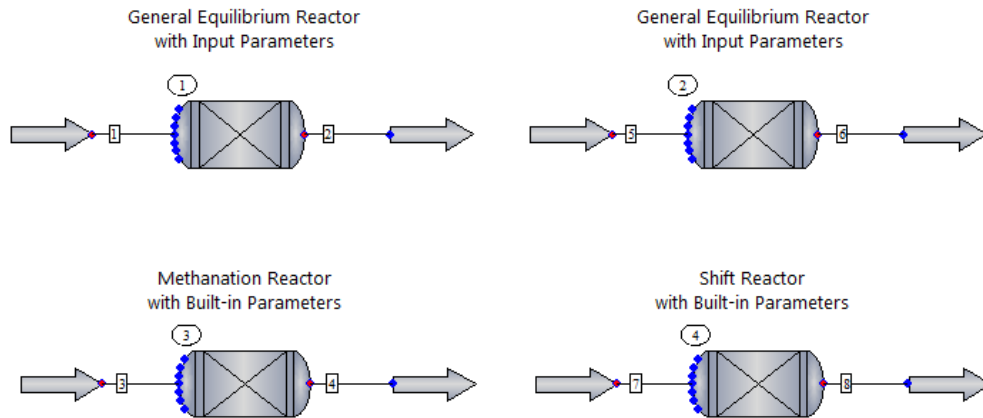
What is the effect of having a larger volume for the kinetic reactors?

What is the effect of having a non-stoichiometric feed?

To learn more about each model, open the relevant specification dialog box, then press **[F1]** to open the appropriate topic in the CHEMCAD help file.

EREA Shift and Methanation Reactors

Comparison between A+B/T and Special methods in CHEMCAD



This simulation compares the resulting equilibrium conversion when changes are made to the feed composition and conditions.

Two of the most common reactions will be evaluated using the Equilibrium Reactor model. Both the water-gas-shift and the methanation reactions occur in the vapor phase.

For these reactions, CHEMCAD has built-in parameters. You can select either the **Shift reactor** or **Methanation reactor** option in the Reactor Model area of the Equilibrium Reactor dialog box.

After you select an option, all the required equilibrium data and stoichiometry for the reaction(s) are stored within the program. These reactions are assumed to take place in the vapor phase.

This example shows how to enter the required data into a general equilibrium reactor (first row) and how to specify the reactor type instead (second row).

The entered equilibrium data is the same that CHEMCAD uses for the shift and methanation reactor. To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Equilibrium Reactor (EREA)."

Methanation
A= -29.3014
B= 26248.4

Water Gas Shift
A= -4.45469
B= 4593.17

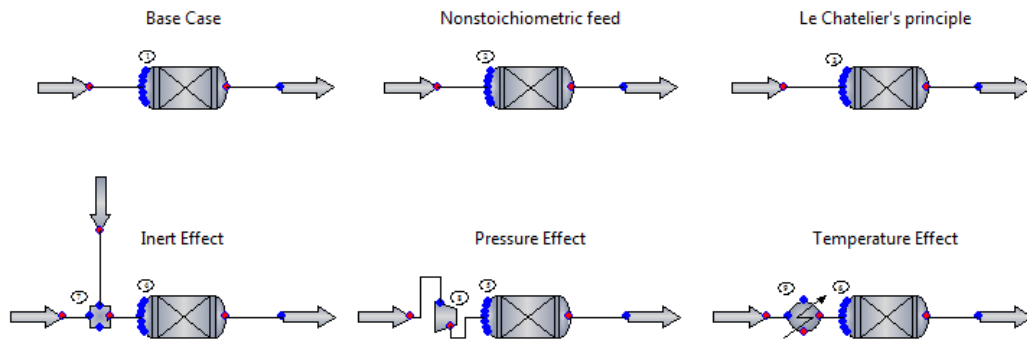
Reaction engineering units:

Temperature: Kelvin
Pressure: ATM
Heat of Reaction: BTU
Molar flow units: Lb-moles

Equilibrium Reactor (EREA)

Water-Gas-Shift Reaction: $\text{CO (g)} + \text{H}_2\text{O (g)} \leftrightarrow \text{CO}_2 \text{(g)} + \text{H}_2 \text{(g)}$

Methanation Reaction: $\text{CO (g)} + 3\text{H}_2 \text{(g)} \leftrightarrow \text{CH}_4 \text{(g)} + \text{H}_2\text{O (g)}$



This simulation compares the resulting equilibrium conversion when changes are made to the feed composition and conditions.

Two of the most common reactions will be evaluated using the Equilibrium Reactor model. Both the water-gas-shift and the methanation reactions occur in the vapor phase.

For these reactions, CHEMCAD has built-in parameters. You can select either the **Shift reactor** or **Methanation reactor** option in the Reactor Model area of the Equilibrium Reactor dialog box.

After you select an option, all the required equilibrium data and stoichiometry for the reaction(s) are stored within the program. These reactions are assumed to take place in the vapor phase.

Note: This example is set for the shift reaction only. To simulate the methanation reactor, include some water in the feed. Also, change the reactor type and change the number of reactions to 2 (both the methanation and water-gas-shift reactions occur here; thus simulation is a multi-reaction equilibria problem).

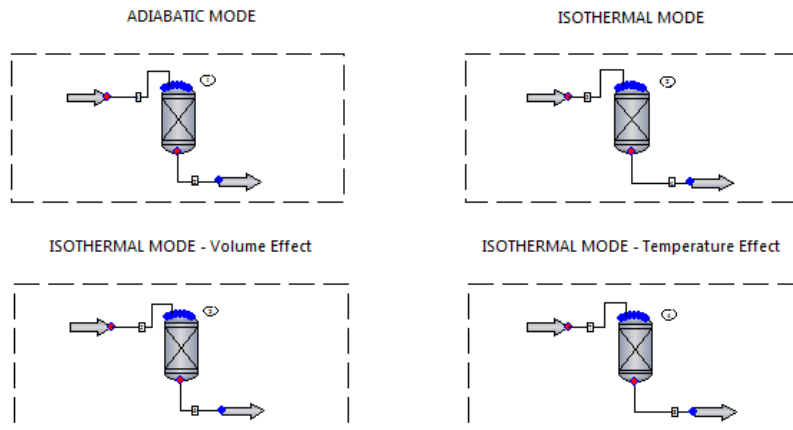
All reactor UnitOps operate isothermally at 826.85 °C. You may choose Adiabatic as the thermal mode when specifying the reactor.

Reference:

Smith J.M., Van Ness, H.C. & Abbott M.M. "Introduction to Chemical Engineering Thermodynamics." Seventh Edition, McGraw-Hill. pp. 483-504, Example 13.5 (modified).

Kinetic Reactor (KREA)

Esterification Reaction: $\text{CH}_3\text{COOH (l)} + \text{C}_2\text{H}_5\text{OH (l)} \rightarrow \text{CH}_3\text{COOC}_2\text{H}_5 \text{ (l)} + \text{H}_2\text{O (l)}$



This example shows an esterification reaction between acetic acid and ethanol to produce ethyl acetate and water using the Kinetic Reactor model. The reaction takes place in the liquid phase. The NRTL K-value has been chosen to model the non-ideal behavior of the mixture.

For this example, the plug flow reactor was chosen as the reactor type. You may switch to a continuous stirred-tank reactor by selecting the option in the Kinetic Reactor dialog box.

The first row shows the difference between the thermal modes. In adiabatic mode, no heat transfer occurs between the reactor and the surroundings. Since this reaction is exothermic, the temperature of the mixture increases, thus vaporizing the mixture. In isothermal mode, the temperature is held constant by adding or withdrawing heat from the reactor. Given the nature of the reaction, heat is removed here.

The second row shows two common ways of improving the yield when using kinetic reactors. Reactor #3 has twice the volume and reactor #4 operates at a higher temperature (70 °C).

Would changing the pressure and/or pressure drop have an effect?

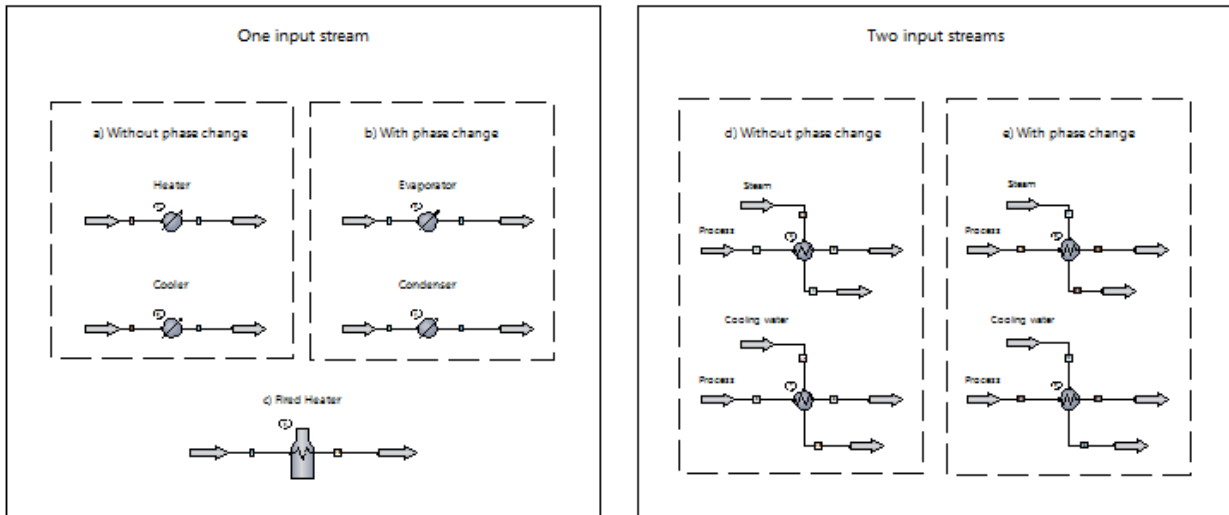
Kinetics of the forward and reverse reactions are considered. The reaction stoichiometry and kinetic data (frequency factor and activation energy) have been entered for each reaction.

Kinetic data were retrieved from Holland, "Fundamentals of Multicomponent Distillation," table B-21.

Review the units for the kinetic expression on the More Specifications tab in the Reactor dialog box.

To learn more about the Kinetic Reactor model, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Kinetic Reactor (KREA)."

Heat Exchangers: Principles and Applications



Heat transfer occurs from a warmer fluid to a cooler fluid through a solid wall separating the two. Heat transfer may be sensible heat—that is, the temperature rises or falls without any phase change—or latent heat, involving a phase change such as condensation or vaporization.

This example focuses on heat exchangers and simple fired heater models.

After running the UnitOp, it is useful to plot a heat curve for the process stream. Go to **Plot > UnitOp Plots > Heat Curves** and choose a plot option. The first option, T vs deltaH, plots temperature as a function of heat duty. The second option, T vs % Length, plots temperature as a function of the % length of the heat exchanger area.

Note: For countercurrent heat exchangers, streams enter the unit from opposite sides.

One input stream:

a) Without phase change (heater or cooler): Specify outlet temperature. CHEMCAD calculates the heat duty (positive for heater) and LMTD correction factor.

Sensible heat is transferred: the fluid is cooled or heated without inducing a phase change. Plot the heat curve and notice the slope of the curve.

b) With phase change (evaporator or condenser): Specify outlet vapor fraction. CHEMCAD calculates the outlet temperature, heat duty, and LMTD correction factor.

Select **Plot > UnitOp Plots > Heat Curves** and notice how the slope flattens as soon as the phase change begins.

c) Fired Heater: Specify outlet temperature. CHEMCAD calculates the heat required and fuel usage to achieve the change in temperature. This UnitOp is used to heat a large amount of material before it enters the process. Optional specifications include the pressure drop and thermal efficiency (default = 75%). The rated heat duty and fuel heating value are specified when a particular fired heater is rated.

Two input streams:

d) Without phase change: The process stream is heated or cooled by using a warmer or colder fluid, respectively. Specify outlet temperature for either stream. CHEMCAD calculates the heat duty (only the positive heat duty is reported) and LMTD. Review the specifications and the heat curves. Plot the heat curves and notice how the slope continuously increases/decreases for one fluid while the other fluid exhibits the opposite trend.

e) With phase change: The process stream is heated or cooled by using a warmer or colder fluid, respectively. Specify outlet temperature for either stream. CHEMCAD calculates the heat duty (only the positive heat duty is reported) and LMTD. Plot the heat curves and notice how the slope flattens during the phase change.

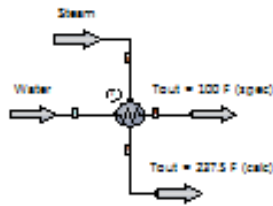
Note: In practice, heat exchangers exhibit a pressure drop. Its magnitude depends on the size of the heat exchanger, as well as the flow rates and temperature change for the streams exchanging heat.

Note: All UnitOps use simulation mode **0 Enter specifications (CHEMCAD simulation)**. With this mode, outlet conditions are calculated based on thermal specifications (e.g., outlet temperature, vapor fraction, heat duty). Ideal heat transfer is calculated according to $Q = U \cdot A \cdot \text{LMTD}$. U is not calculated rigorously. To use any of the other terms, you need to have a CC-THERM license.

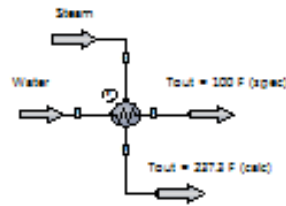
To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics called "Simple Heat Exchanger" and "Two-sided Heat Exchanger."

Heat Exchangers: Use Cases

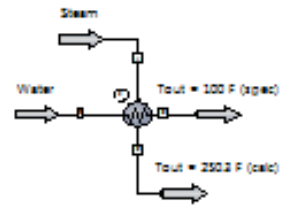
1 (base case) - specify T out



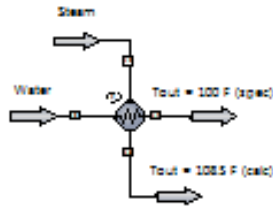
2 - pressure drop specified



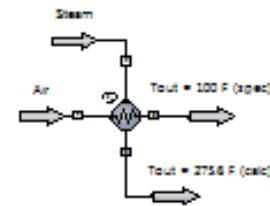
3 - steam at higher P



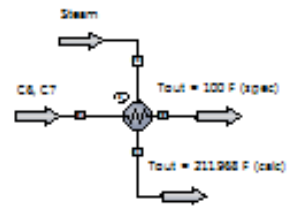
4 - with phase change



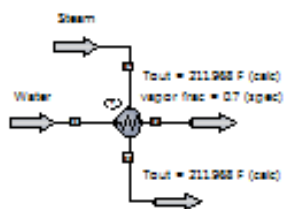
5 - air (lower heat capacity)



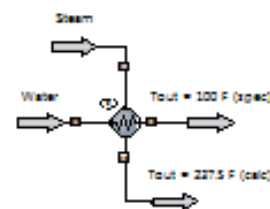
6 - C6 and C7 (higher heat capacity)



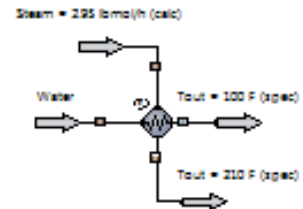
7 - vapor fraction specified



8 - larger utility flowrate



9 - calculate utility flowrate



Heat transfer occurs from a warmer fluid to a cooler fluid through a solid wall separating the two. Heat transfer may be sensible heat—that is, the temperature rises or falls without any phase change—or latent heat, involving a phase change such as condensation or vaporization.

This example demonstrates the use of the two-sided heat exchanger. For all cases, steam at 300 °F is the utility stream.

Notice the outlet temperature for the utility in all cases. What do you observe?

After running the UnitOp, it is useful to plot a heat curve for the process stream. Go to **Plot > UnitOp Plots > Heat Curves**, and select either of the two plot options. The first option, T vs ΔH , plots temperature as a function of heat duty. The second option, T vs % Length, plots temperature as a function of the % length of the heat exchanger area.

Note: For countercurrent heat exchangers, as in this example, streams enter the unit from opposite sides.

Notice the slope for each fluid in the heat curve. Is the slope the same? Does the slope change at any point?

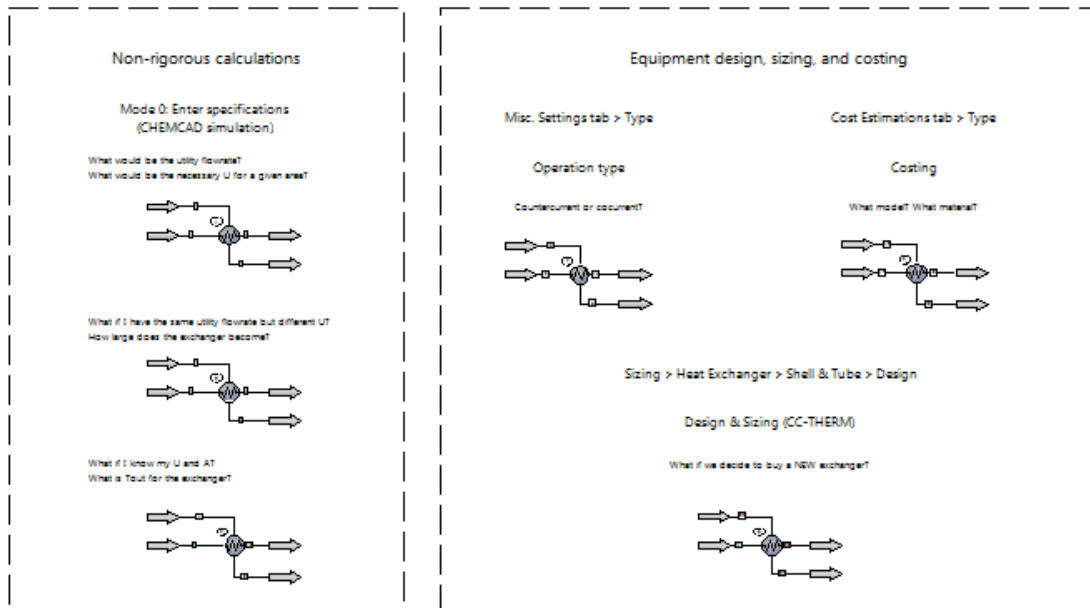
Note: Heat exchangers on this flowsheet use simulation mode **0 Enter specifications (CHEMCAD simulation)**. With this mode, outlet conditions are calculated based on thermal specifications (e.g., outlet temperature, vapor fraction, heat duty). Ideal heat transfer is

calculated according to $Q = U \cdot A \cdot \text{LMTD}$. U is not calculated rigorously. To calculate U rigorously from geometry, you need to have a CC-THERM license.

All cases with the exception of case 9 have the utility option turned off. When the utility option is activated (UnitOp 9), CHEMCAD adjusts the flow rate of an input stream, in this case the utility, to match the required duty (calculated) of the unit. Using this option requires two specifications (e.g., outlet temperature for each stream), instead of only one as in cases 1-8.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics called "Simple Heat Exchanger" and "Two-sided Heat Exchanger."

Heat Exchangers: Equipment Design, Sizing, and Costing



After running the UnitOp, it is useful to plot a heat curve for the process stream. Select **Plot > UnitOp Plots > Heat Curves**, and select either of the two plot options. The first option, T vs ΔH , plots temperature as a function of heat duty. The second option, T vs % Length, plots temperature as a function of the % length of the heat exchanger area.

Note: For countercurrent heat exchangers, as in this example, streams enter the unit from opposite sides.

Notice the slope for each fluid in the heat curve. Is the slope the same? Does the slope change at any point?

This example shows the various simulation modes for a two-sided heat exchanger.

Simulation mode 0 calculates outlet conditions non-rigorously, while modes 1-6 do so rigorously. The use of these modes requires a CC-THERM license.

(1) T for stream 2 and vapor fraction for stream 4 specified, as well as the pressure drop for both streams. Area (per shell) is specified, thus the heat transfer coefficient U is calculated. With the selected utility option, CHEMCAD calculates the utility flow rate (stream 3).

(2) Stream 7 is specified with the same steam flow rate as Stream 3. The heat transfer coefficient U is specified (but different from the one calculated for UnitOp 1), thus the area (per shell) is calculated.

(3) Both U and area (per shell) are specified. This counts as a single thermal specification and the dialog box is complete. The outlet temperatures are calculated for both streams.

(4) Cocurrent has been selected as the exchanger type in the Misc. Settings tab. Countercurrent is most common due to its higher efficiency. You can change the flow rate of water to 9000 kg/h, run the UnitOp, and then select **Plot > UnitOp Plots > Heat Curves > Plot X-axis = % Length** to appreciate the difference.

(5) Additional specifications can be entered under the Cost Estimations tab. The option to run the costing report has been checked for this UnitOp.

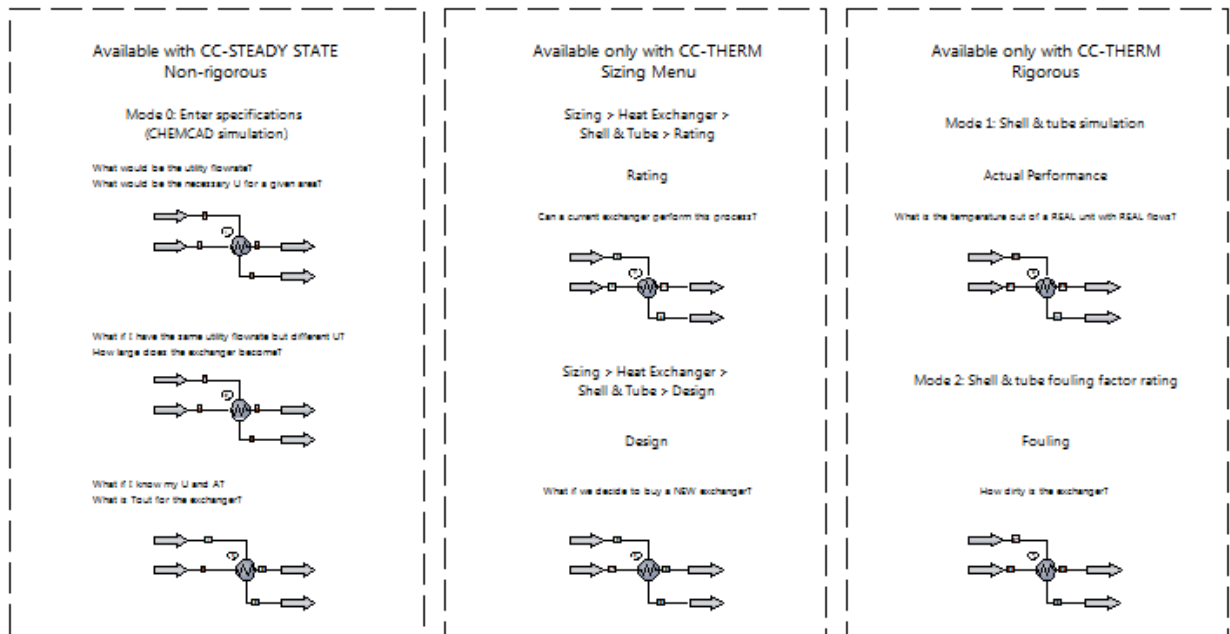
(6) Design mode gives us an exchanger design, based on flowsheet performance as a requirement.

Select **Sizing > Heat Exchanger > Shell & Tube** to bring up the Shell and Tube Exchanger menu. For this example, no specifications have been entered in the tabs, so the default settings and values are used for the calculation. Click **General Specifications** and change the Calculation Mode setting to **Design**.

For results, click **View Results** and then **Summary Results**.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics called "Two-sided Heat Exchanger" and "Shell and Tube Overview."

Heat Exchangers: CC-THERM Modes



This example shows the various simulation modes for a two-sided heat exchanger.

Mode 0 calculates outlet conditions non-rigorously, while modes 1-6 do so rigorously. The use of these modes requires a CC-THERM license.

(1) T for stream 2 and vapor fraction for stream 4 specified, as well as the pressure drop for both streams. Area (per shell) is specified, thus the heat transfer coefficient U is calculated. With the selected utility option, CHEMCAD calculates the utility flow rate (stream 3).

(2) Same flow rate as stream 3 is specified for stream 7. The heat transfer coefficient U is specified (but different than the one calculated for UnitOp 1), thus the area (per shell) is calculated.

(3) Both U and area (per shell) are specified. This counts as a single thermal specification and the dialog box is complete. The outlet temperatures are calculated for both streams.

(4) Rating mode shows us "Can our exchanger give us flowsheet performance?"
 Select **Sizing > Heat Exchangers > Shell & Tube > General Specifications**, and set Calculation mode to **Rating**. This example uses the default values in the Shell and Tube Exchanger menu.

For CC-THERM:

Effective Area is "How much area does this unit have for heat transfer?"

Area required is "How much area does the unit require to perform the specified heat transfer?"

Ucalc is based on rigorous calculation of heat transfer.

Ucalc is calculated from $Q=U \cdot A \cdot \text{LMTD}$ using required area, outlet temperatures, and overall duty.

Ucalc represents the apparent heat transfer of the unit.

Uservice represents the heat transfer that would occur if you observe this unit performing as specified.

Uservice is calculated from $Q=U \cdot A \cdot \text{LMTD}$ using effective area, outlet temperatures, and heat specification for the unit.

In general, if $U_{calc} < U_{service}$, the exchanger is not capable of performing the desired heat transfer.

(5) Design mode gives us an exchanger design, based on flowsheet performance as a requirement. Select **Sizing > Heat Exchangers > Shell & Tube > General Specifications**, and set Calculation mode to **Design**. This example uses the default values in the Shell and Tube Exchanger menu.

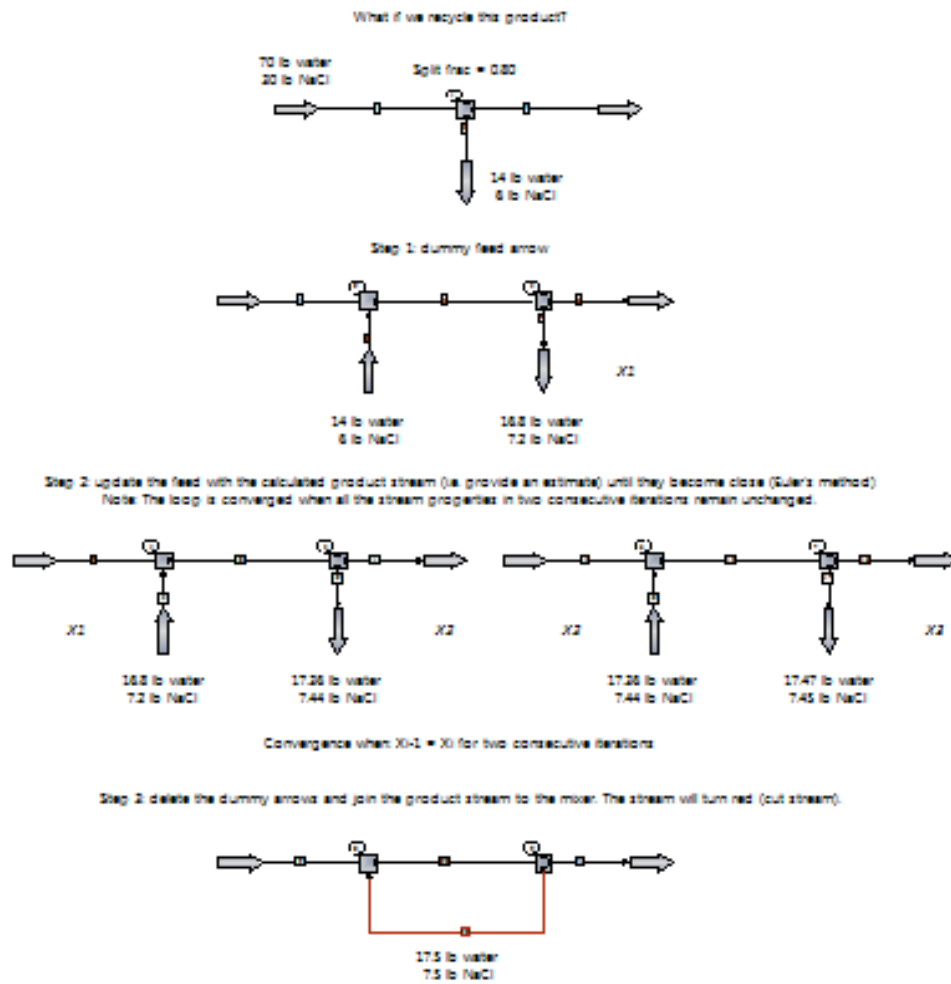
(6) Simulation mode lets you answer the question: "What would happen if these feeds went through this CCT exchanger?"

(7) The fouling rating lets you change the fouling until the predicted temperatures out-match reality.

We know the temperatures out, and the geometry.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics called "Two-sided Heat Exchanger" and "Shell and Tube Overview."

Recycle: Closing the Loop

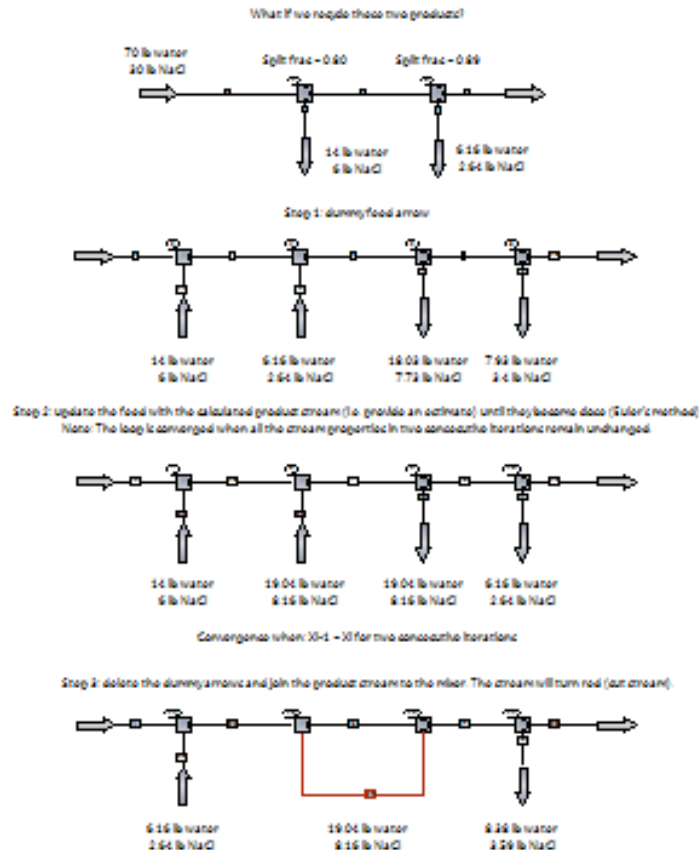


CHEMCAD can automatically handle recycle problems by determining recycle cut streams and unit operation calculation sequence.

Select **Run > Convergence Parameters** to review the default settings and/or make changes. Smart Cut allows for faster convergence, but you can choose Normal recycles if you prefer.

You can override this and specify your own cut streams by selecting **Specifications > Select Cut Streams**. You need to make sure that they cut the recycle loops completely.

Nested Recycle: Closing the Inner Loop

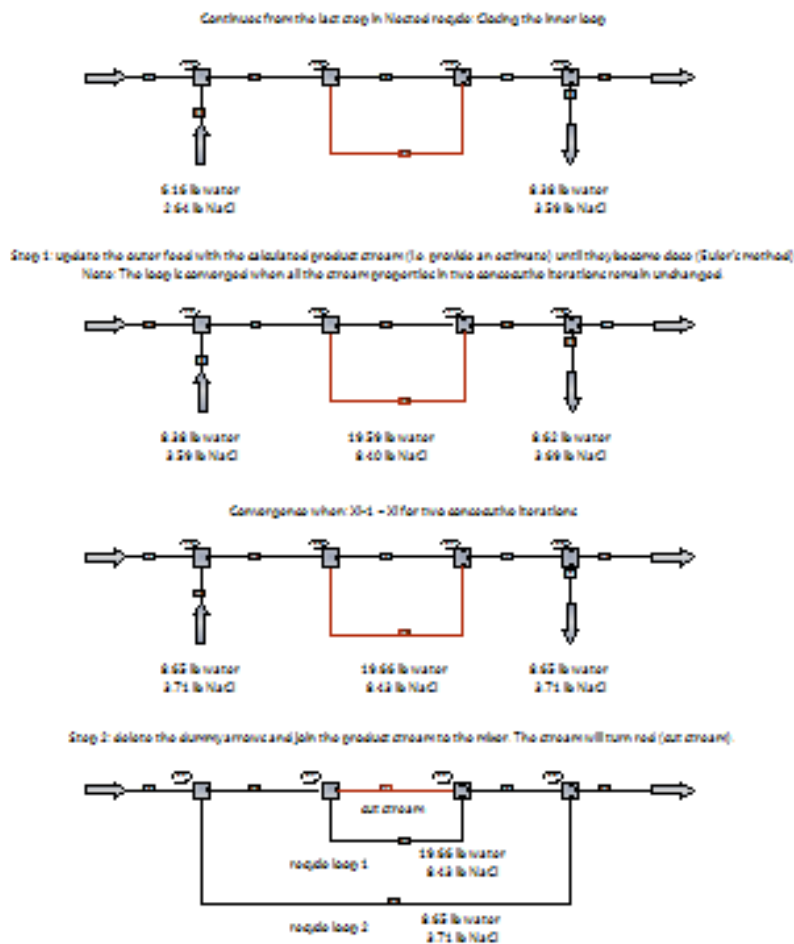


CHEMCAD can automatically handle recycle problems by determining recycle cut streams and unit operation calculation sequence.

Select **Run > Convergence Parameters** to review the default settings and/or make changes. Smart Cut allows for faster convergence, but you can choose Normal recycles if you prefer.

You can override this and specify your own cut streams by selecting **Specifications > Select Cut Streams**. You need to make sure that they cut the recycle loops completely.

Nested Recycle: Closing the Outer Loop

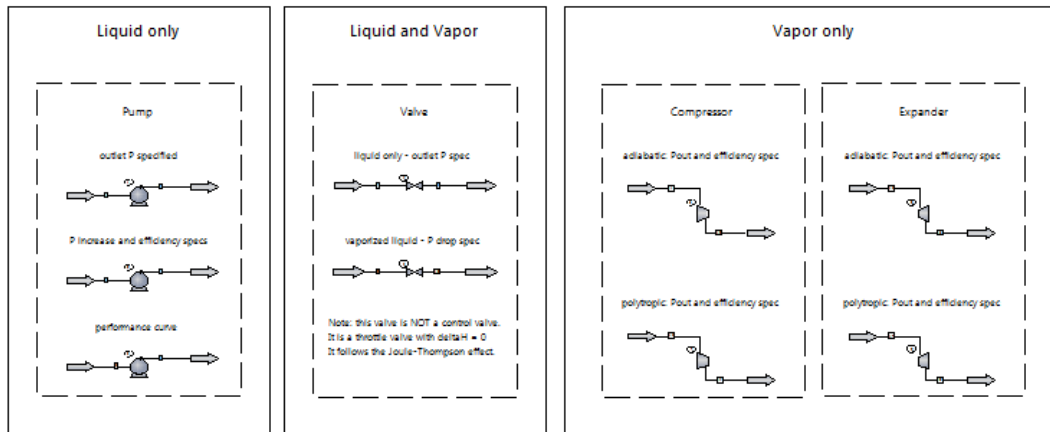


CHEMCAD can automatically handle recycle problems by determining recycle cut streams and unit operation calculation sequence.

Select **Run** > **Convergence Parameters** to review the default settings and/or make changes. Smart Cut allows for faster convergence, but you can choose Normal recycles if you prefer.

You can override this and specify your own cut streams by selecting **Specifications** > **Select Cut Streams**. You need to make sure that they cut the recycle loops completely.

Flow Models: Input Specifications



This example shows the equipment used to change the pressure of the fluids in a process.

Pumps increase the pressure of a liquid stream. When you specify discharge pressure or pressure increase, CHEMCAD calculates the required work. If efficiency is not specified, ideal work is calculated (efficiency = 1). Notice how lower efficiency causes the temperature of the liquid to increase. This is because the additional work (compared to the ideal) goes into the fluid. Pumping liquid is cheap, and the properties of the fluid are not changed by much. If there is vapor inside the pump, CHEMCAD will issue a warning and the pump ID will turn yellow.

Valves decrease the pressure of a fluid, either liquid, vapor, or saturated mixture. The valve performs an adiabatic flash calculation on the inlet stream at output pressure. The Joule-Thomson effect describes the temperature change of a fluid as it expands through the valve. The change in enthalpy is zero and no work is produced. Notice the outlet temperature of the streams.

Compressors increase pressure of a vapor stream. The model type (adiabatic or polytropic), output pressure, and efficiency (relative to isentropic operation) need to be specified. CHEMCAD then calculates the required work. Both the theoretical and actual power are calculated. Notice that the temperature increases. Is there any difference between the adiabatic and polytropic mode? Compressors are expensive. If there is liquid in the inlet, CHEMCAD will issue a warning and the compressor ID will turn yellow. A flash drum is usually placed downstream to separate any liquid from the stream.

Expanders perform the opposite operation by expanding the gas, lowering its temperature, and generating power as a result.

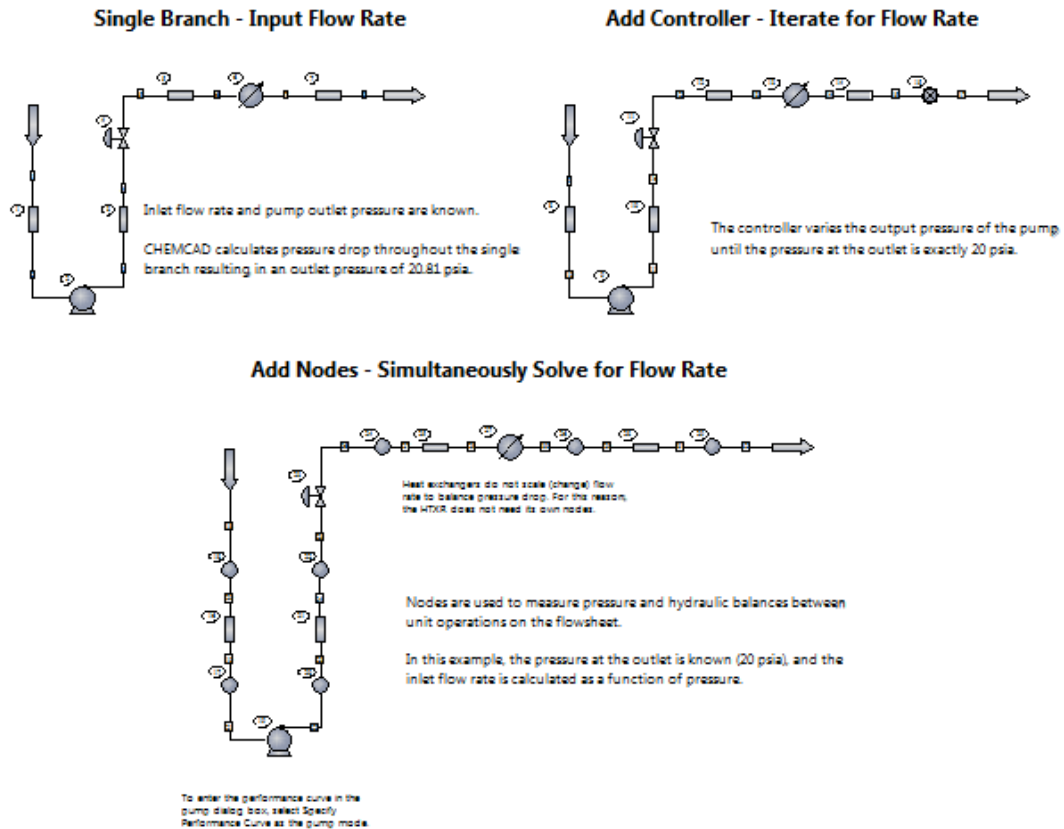
Using the **Specify performance curves** mode for either the pump or the compressor/expander allows you to enter the performance curve for the equipment. **Specify performance curve** is selected as the UnitOp mode, the speed lines and pump speed specified, and the curve data entered on the appropriate column of the matrix that appears when you click **OK**. This option allows for pressure-flow balance methods to be used.

Two options: 1) **Fixed flow rate, calculate Pout** (used in this example) calculates the outlet pressure considering the inlet flow rate and the performance curve data; 2) **Pout from downstream uop, calc flow rate** (see Single branch piping example) requires a downstream unit operation such as a Node UnitOp that would set the suction pressure. CHEMCAD then calculates the flow rate passing through the pump. This is used to perform hydraulic balance on piping systems.

Equipment costing: On the Cost Estimation tab of the UnitOp dialog box, you can enter additional specifications, then click **Run the costing report after calculating unit**.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topics for the Compressor/Expander, Liquid Pump, and Valve UnitOps, found under **UnitOps and Other Flowsheet Objects > UnitOps > Piping and Flow**.

Single-branch Piping Configurations



Single Branch – Input Flow Rate:

Inlet flow rate and pump outlet pressure are known. CHEMCAD calculates pressure drop throughout the single branch, resulting in an outlet pressure of 20.81 psia.

Add Controller – Iterate for Flow Rate:

The controller varies the output pressure of the pump until the pressure at the outlet is exactly 20 psia.

Add Nodes – Simultaneously Solve for Flow Rate:

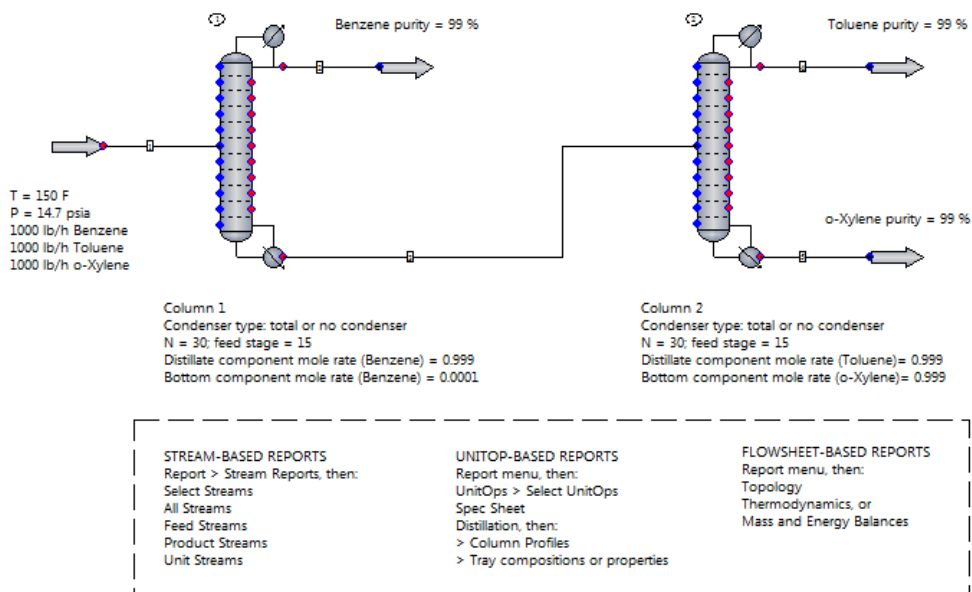
Heat exchangers do not scale (change) flow rate to balance pressure drop. For this reason, the heat exchanger does not need its own nodes.

Nodes are used to measure pressure and hydraulic balances between unit operations on the flowsheet.

In this example, the pressure at the outlet is known (20 psia), and the inlet flow rate is calculated as a function of pressure.

To enter the performance curve in the pump dialog box, select Specify Performance Curve as the pump mode.

Reports: Benzene/Toluene/Xylene Distillation



In this simulation, a mixture of benzene, toluene, and o-xylene is separated to produce three product streams, each at least 99.9 mole % pure. To learn how to build this flowsheet, see the example called **_Process Simulation Essentials\3 Separators\3 – Distillation column design**.

The purpose of this example is to show the reports that CHEMCAD generates and how to access them. Follow the instructions below to generate individual reports.

Report output setup:

To choose how to display reports, select **Tools > Options > Preferences**, then click **Report Viewer**. Change the default report viewer by choosing among CHEMCAD's internal report viewer, MS Word, MS Excel, and others. Click **OK**.

Stream-based reports:

First, select the Stream Composition property set by selecting **Report > Stream Reports > Select Active Property Set > Stream Composition**. Then select **Report > Stream Reports** and choose either **Select Streams** (type in the stream IDs one per line or click on the streams), **All Streams**, **Feed Streams**, **Product Streams**, or **Unit Streams** (inlet and outlet streams for a specified UnitOp).

To customize the stream properties that appear on the report, you can select **Report > Stream Reports > Customize Property Sets**. Click **Help** on the Property Set Preferences dialog to learn more about property sets and customizing stream reports.

Tip: Right-click a stream in the flowsheet, then select **Stream Reports > Stream Composition** to quickly display stream composition data.

Note: These reports will use the flowsheet engineering units. To change units for reporting, select **Format > Engineering Units > Options and references**, then choose an option in the **Legacy flow units** drop-down box.

UnitOp-based reports:

Select **Report > UnitOps > Select UnitOps**, then enter the stream IDs one per line or click on the UnitOp symbols.

Spec Sheet: Select **Report > Spec Sheet** to export detailed information into a pre-formatted Excel worksheet (one per piece of equipment). This is useful for soliciting a manufacturing quote, for example.

Distillation: Select **Report > Distillation**, then select either: 1) Column Profiles (T, P, and flow rate for a column); 2) Tray Compositions (vapor and liquid flow rate, and K-value of each component on each stage); 3) Tray Properties (currently selected stream properties for each stage).

Flowsheet-based reports:

Select **Report > Topology** to list all UnitOps, streams origins and destinations.

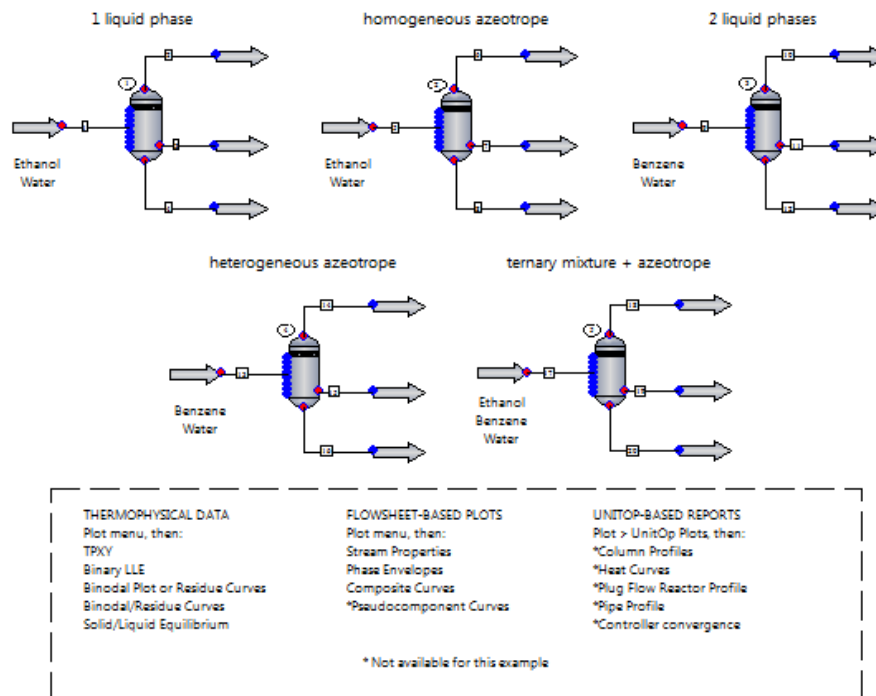
Select **Report > Thermodynamics** to list all components and thermodynamics used (K-value, enthalpy model, and BIPs).

Select **Report > Mass and Energy Balances** to view mass and energy balances as well as information about the calculation mode used, convergence, recycle loops, and cut streams, if any.

You can also customize a combination of individual reports. Select **Report > Consolidated Report**, then select the sections of interest and generate the report.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Output and Reports."

Plots: Thermophysical Data



The purpose of this example is to show the plots that CHEMCAD generates and how to access them.

Note: Plots marked with an asterisk are not available using this example. The feed streams and Flash UnitOps have been specified to provide representative examples. Review the specifications and resulting product streams. To learn more, see the examples in the Phase Equilibria folder.

For each feed stream:

Select the stream, then go to the **Plot** menu and select:

- 1) **TPXY** to generate TXY, PXY, and XY diagrams. Specify binary mixture and either constant T or P. It's most common to select the more volatile component first.
- 2) **Binary LLE** to generate liquid-liquid equilibrium curves between any two components. An activity coefficient method should be selected as the K-value model and Vapor/Liquid/Liquid/Solid should be selected as the Global Phase Option (see **Thermophysical > Thermodynamic Settings > K-value models**).

- 3) **Solid/Liquid Equilibrium** to generate solid-liquid equilibrium curves between any two components. Vapor/Liquid/Liquid/Solid should be selected as the Global Phase Option (see **Thermophysical > Thermodynamic Settings > K-value models**).

For stream 17 only (because the mixture is ternary and benzene and water form two liquid phases):

- 4) **Binodal Plot** to generate a ternary phase diagram that shows the component distribution in the two liquid phases. Enter the ternary mixture and temperature.

5) **Residue Curves** to display distillation zones, azeotropes, and residue curves. Specify ternary mixture and pressure.

6) **Binodal/Residue Curves** combines the curves from a binodal plot and residue curve plot. This is useful for heterogeneous azeotropic distillation. The order in which you select the components determines the edges of the equilateral triangle chart.

For a binodal plot: The first component becomes the left edge, the second component the right edge, and the third component the base. The first and third components should form two liquid phases.

For binodal/residue curve and residue curve plots: The first component becomes the base, the second component the right edge, and the third component the right edge.

Note: The first and third components should form two liquid phases.

Flowsheet-based plots:

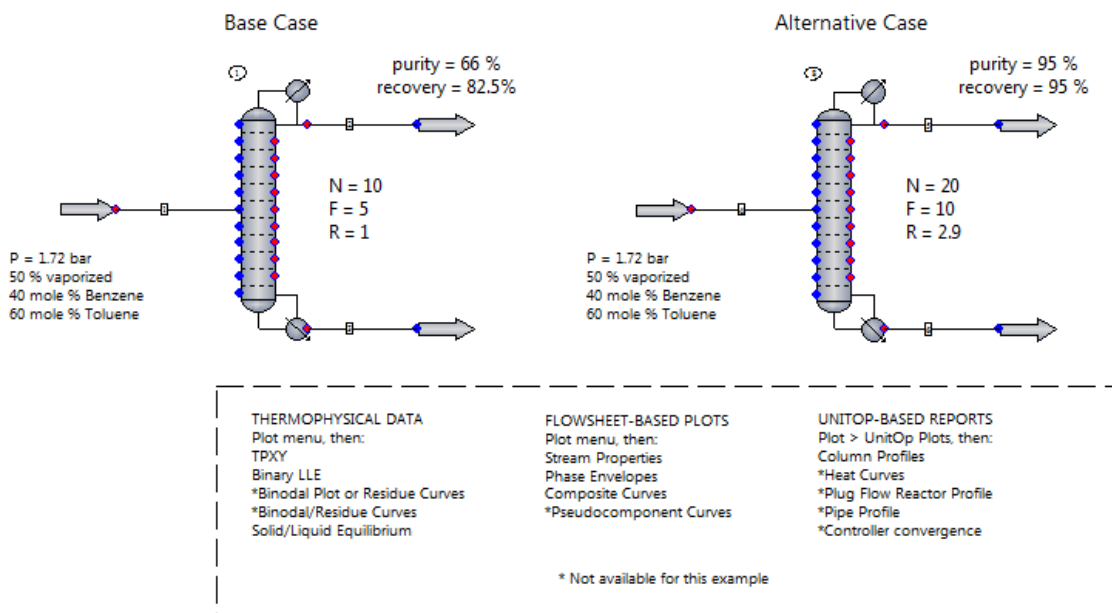
Select the stream, then go to the **Plot** menu and select:

1) **Stream Properties** to plot one selected stream property (e.g., vapor pressure, density, viscosity) as a function of temperature. Specify the temperature range, then click **OK**.

2) **Phase Envelopes** to plot a phase envelope. The text report includes tabulated data and T_c, P_c, Z_c values for the mixture. The critical point of the mixture is indicated. Plots at vapor fractions other than 0 and 1 can be included.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Output and Reports." The "Graphical Reports" section of this topic addresses plots.

Plots: Benzene/Toluene Distillation



In this example, a mixture of benzene and toluene is separated by distillation. The Tower distillation model was used to perform rigorous calculations. The two columns shown have different specifications and performance.

To learn how to build this example, see the example called **_Process Simulation Essentials\3 Separators\4 – Distillation column performance**. The purpose of this example is to show the plots that CHEMCAD generates and how to access them.

Note: Plots marked with an asterisk are not available using this example.

Select stream 1, then **Plot > TPXY**. Generate TXY, PXY, and XY diagrams. Specify the binary mixture and either constant T or P. It's most common to select the more volatile component first.

Select stream 1, then **Plot > Binary LLE**. CHEMCAD will tell you that benzene and toluene are miscible, and thus only one liquid phase exists.

The Binodal plot is not available because these components do not form two liquid phases. The Residue Curves plot is not available because this is a binary mixture.

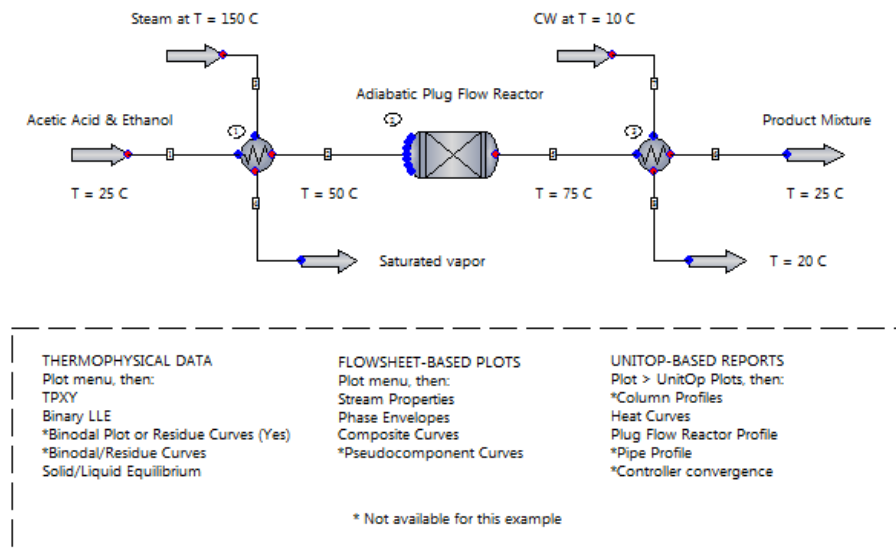
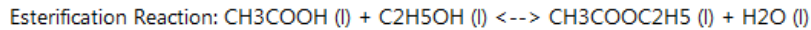
Select stream 1, then **Plot > Solid/Liquid Equilibrium**. Enter the binary mixture.

Select either column, then **Plot > Composite Curves** to get a plot of T vs Delta H for both the condenser and reboiler.

Select either column, then **Plot > UnitOp Plots > Column Profiles** and customize the plot.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Output and Reports." The "Graphical Reports" section of this topic addresses plots.

Plots: Exchangers and Plug Flow Reactor



In this example, acetic acid and ethanol react to form ethyl acetate and water according to the reversible esterification reaction. The reaction takes place in the liquid phase, and the NRTL K-value has been chosen to model the non-ideal behavior of the mixture.

In addition, the Plug Flow Reactor was chosen as the reactor type. The purpose of this example is to show the plots that CHEMCAD generates and how to access them.

Note: Plots marked with an asterisk are not available using this example.

Select stream 1, then **Plot > TPXY**. Generate TXY, PXY, and XY diagrams. Specify the binary mixture and either constant T or P. It's most common to select the more volatile component first.

Select stream 1, then **Plot > Binary LLE**. CHEMCAD will tell you that acetic acid and ethanol are miscible, and thus only one liquid phase exists.

The Binodal plot is not available because these components do not form two liquid phases.

Select stream 5, then **Plot > Residue Curves**. Enter the ternary mixture and specify pressure.

Select stream 6, then **Plot > Solid/Liquid Equilibrium**. Enter any two components.

For both heat exchangers, the utility option is active, allowing CHEMCAD to determine the utility flow rate provided two thermal specifications. The first heat exchanger is specified as countercurrent, while the second is specified as cocurrent (Heat Exchanger dialog box > **Misc. Settings > Type**).

The heat curve will change depending on what type is selected. **Plot > UnitOp Plots > Heat Curves**, select the plot option, and obtain a heat curve for each heat exchanger. For more on heat exchangers, see the examples in **_Process Simulation Essentials\5 Heat Exchangers**.

The Plug Flow reactor is adiabatic, so no heat transfer occurs between the reactor and the surroundings. Since this reaction is exothermic, the temperature of the mixture increases.

Kinetics of the forward and reverse reactions are considered. The reaction stoichiometry and kinetic data (frequency factor and activation energy) have been entered for each reaction.

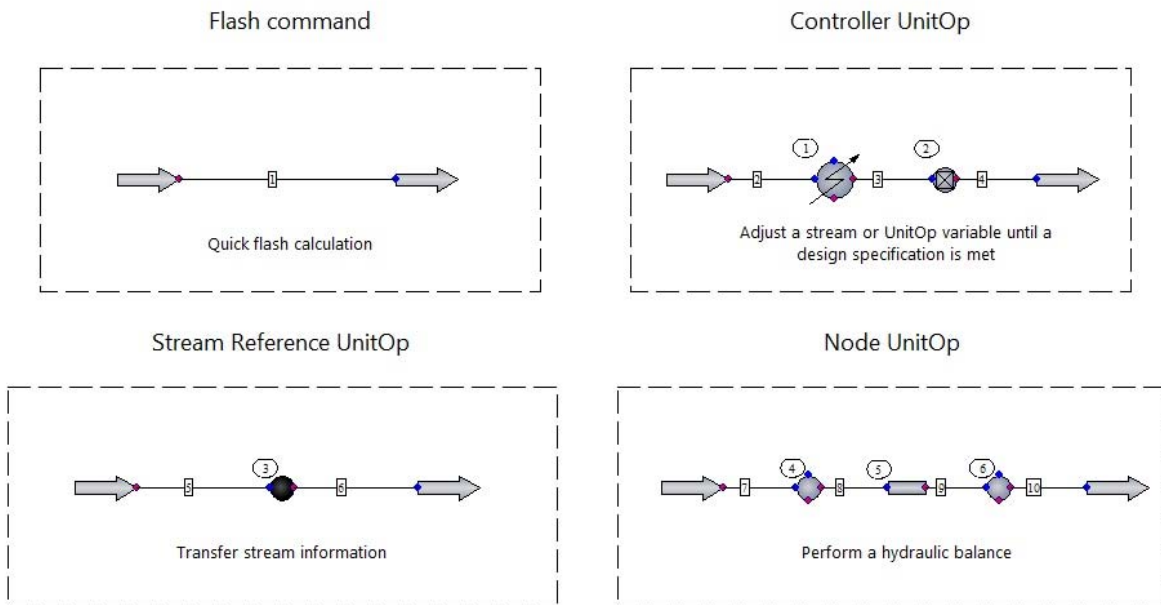
Kinetic data was retrieved from Holland, "Fundamentals of Multicomponent Distillation," table B-21.

Review the units for the kinetic expression by clicking the **More Specifications** tab in the Reactor dialog box. For more on reactors, see the examples in **_Process Simulation Essentials\4 Reactors**.

Go to **Plot > UnitOp Plots > Plug Flow Reactor Profile** and select the components and independent variable of interest. For example, plot moles of both acetic acid (reactant) and ethyl acetate (product) vs reactor volume (axial length), and include temperature (check the option).

To learn more about plots, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Output and Reports." The "Graphical Reports" section of this topic addresses plots.

Tools: UnitOps



This example shows several of CHEMCAD's utility tool UnitOps, which are used in building and running flowsheets. Familiarize yourself with basic use of CHEMCAD as demonstrated in the earlier CHEMCAD Essentials examples before using these UnitOps.

Flash command (at a stream):

The **Flash** button on a stream dialog allows for a quick flash calculation. Define the stream by specifying composition and two variables (T, P, or vapor fraction), then click the **Flash** button located at the upper left corner of the Edit Streams dialog box. For example, specify Stream 1 vapor fraction = 0.5 and P = 1 bar. Clicking **Flash** will show you the temperature at this condition. Transport properties can be seen in the stream properties report, or by hovering over the stream line with the Flowsheet Quickview feature turned on.

Feed-backward and Feed-forward Controller UnitOp:

In Feed-backward mode, the controller behaves as a solver routine. In this example, the controller (UnitOp 2) adjusts the thermal specification inside the heater (i.e., temperature out) until the vapor fraction of stream 3 is 50% vaporized. The controller will change the adjusted variable and run UnitOps until stream 3 reaches the 50% vapor target, then determine if the solution has been found.

In Feed-forward mode, the Controller UnitOp allows a variable to be transferred forward to another location on the flowsheet.

To learn more, click the **Help** button in the Controller dialog box, or see the controller examples in **_Process Simulation Essentials\9 Tools**. A separate PID controller UnitOp is available for dynamic simulations.

Stream Reference UnitOp:

This UnitOp can transfer stream information to another process stream. It should be placed downstream of the UnitOp that calculates the information to be passed. Various modes and

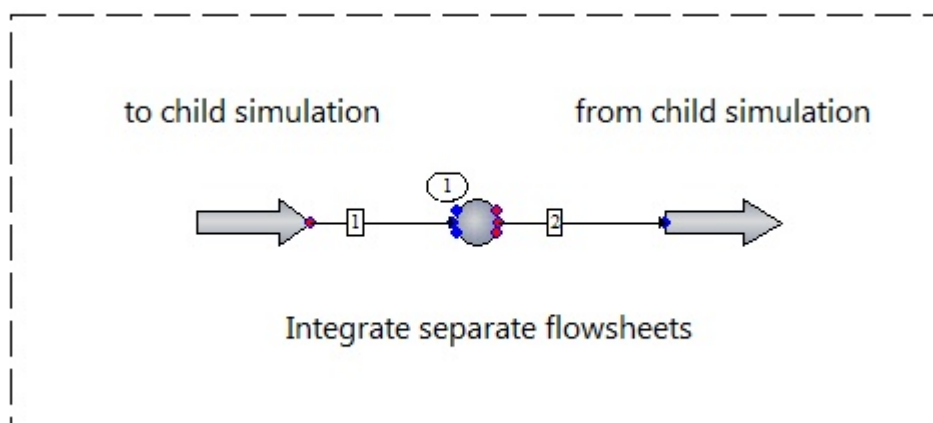
transfer options are available, which can be reviewed by clicking the **Help** button in the Stream Reference dialog box.

For this example, the stream reference passes stream information from stream 7 to stream 9. Alternatively, specify stream 6 as the source stream number in the Stream Reference dialog box and see the resulting outlet pressure when the stream flow rate and temperature are different.

Node UnitOp:

Nodes are used to measure pressure and perform hydraulic balances between unit operations on the flowsheet. They are placed upstream and downstream of pipes, pumps, and control valves in piping systems. To learn more, see the examples located in **_Process Simulation Essentials\7 Pressure**. For this example, the nodes facilitate the calculation of the pressure drop across the pipe.

Tools: META UnitOp



This example shows CHEMCAD's UnitOp tools, which are used in building and running flowsheets. We do not recommend using these tools if you have only recently started using CHEMCAD.

It is not unusual for multiple flowsheets to model various parts of a process. Integrated flowsheets may be too large and complicated to handle. In addition, these flowsheets may have different components and thermodynamics. The subflowsheet unit operation (META UnitOp) sends stream data to a second flowsheet (child simulation), runs it, and returns data to the parent flowsheet.

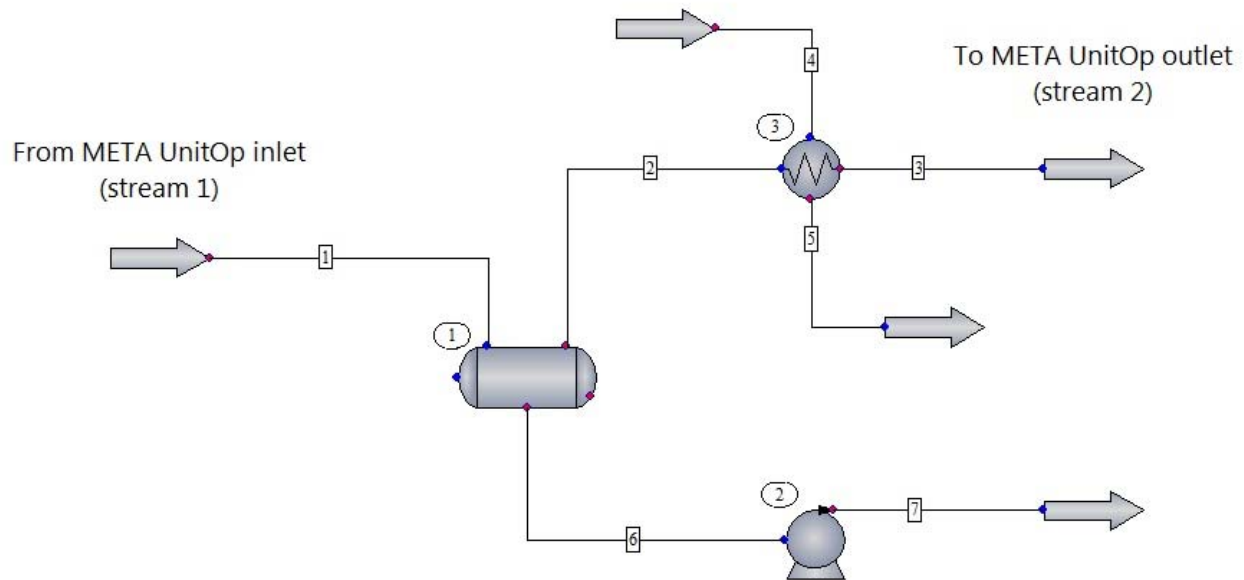
The child flowsheet created for use with this simulation is located in **_Process Simulation Essentials\9 Tools**.

The META UnitOp requires the specification of inlet and outlet streams for both the parent and child simulations, as well as the path for the child simulation, which you can generate by browsing for the file of interest.

To learn more, press **[F1]** to open the CHEMCAD help file, then see the help topic called "Subflowsheet Unit Operation (META)."

Note: The META UnitOp can only run using the sequential modular calculation sequence. Select **Run > Convergence Parameters** to change the calculation sequence setting.

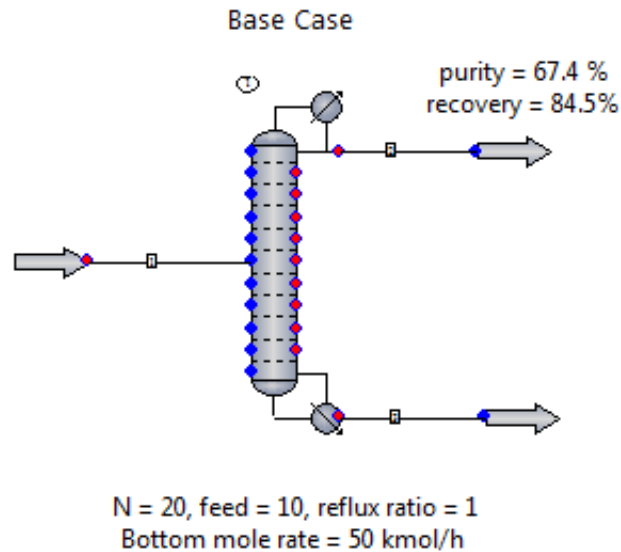
Tools: Child Simulation for META UnitOp



The purpose of this flowsheet is to serve as the child simulation for the META UnitOp in the UnitOp Tools example.

The META UnitOp defines the feed stream, runs this simulation, and sends the product stream (stream 3) back to the parent flowsheet.

Tools: Sensitivity Study



In this example, a mixture of benzene and toluene is separated by distillation. The Tower distillation model is used to perform rigorous calculations. The goal is to obtain the highest benzene purity and recovery in the distillate.

Purity = benzene mole fraction.

Recovery = mole rate benzene in distillate/mole rate benzene in feed.

Base case column is designed as follows:

Condenser type: Total or no condenser

Number of stages (N) = 20

Feed stage (F) = 10

50 % vaporized feed

Pressure = 1.72 bar (constant)

Reflux Ratio (R) = 1

Bottoms mole rate (B) = 50 kmol/h

The next step is to investigate the effect of changing a parameter or specification. This activity can be carried out automatically using the Sensitivity Study feature. Sensitivity studies help us investigate the best parameters for a column that has 20 stages.

Note: This tool enables you to test multiple cases efficiently, but it does not give you the optimum answer. However, the reports and plots can help you decide the best operation based on design specifications, operational constraints, or economics.

To load a sensitivity study, select **Run > Sensitivity Study > [study name] > Run All**.

To review the input, select **Run > Sensitivity Study > [study name] > Edit**.

To review the results, select **Run > Sensitivity Study > [study name] > Report Results or Plot Results**.

The sensitivity studies are explained next:

The study called "FeedLoc" records the mole fraction and mole rate of benzene in the distillate as the feed location is changed from $N = 2$ to $N = 19$ in equal steps.

The study called "Reflux" varies the reflux ratio from 1 to 15 in equal steps. It records the condenser and reboiler duties, as well as the mole fraction and mole rate of benzene in the distillate.

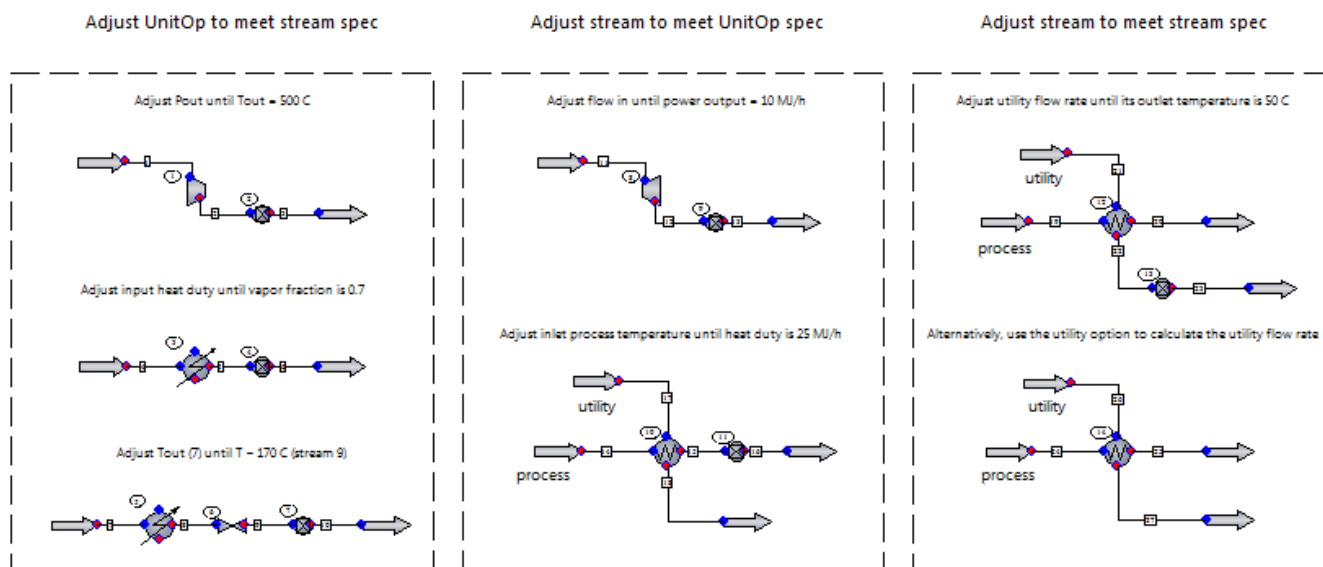
The study called "2variables" varies the pressure drop across the column from $\Delta P = 0$ to $\Delta P = 5$ bar. It also varies the specification for the reboiler, that is, the bottom mole rate from 10 to 70 kmol/h. The study then records the temperature of stream 3 (bottom), and the mole fraction and mole rate of benzene in the distillate.

Note: Each independent variable is treated separately. This tool cannot find correlations between the parameters. This sets the bottom flow rate at 10 kmol/h and varies the pressure drop. Then it changes to 20 kmol/h and repeats for each value of pressure drop.

After running the sensitivity studies, click **Yes** to reset process data to the original state; otherwise, the value of the last run will override the original specification for the column.

To obtain a summary of results for the column(s), select **Report > UnitOps > Select UnitOps**. For tabulated results, right-click the UnitOp and select **View Column Profile**. Select **Plot Column Profile** from the right-click menu to generate plots for the temperature profile, total vapor flow, and/or total liquid flow.

Controller: Simple Applications



The Controller UnitOp behaves as a solver routine. The feed-backward mode, shown in this example, adjusts one variable (from an equipment or a stream) until the measured variable equals the setpoint. Scaling is allowed. The setpoint can be an algebraic calculation of two measurements.

In other words, the controller compares the measured variable to a setpoint and decides a new value for the adjusted variable until the specified condition is achieved.

The General Settings tab's information flow is as follows:

Adjust this variable . . .

Until this . . .

Is equal to this target.

Adjust this variable: Specify UnitOp or stream ID, the adjusted variable and its unit, and the lower and upper bounds (do not enter if you are not sure).

Until this: Specify UnitOp or stream ID, the specification variable, and any scaling or arithmetic operation (optional).

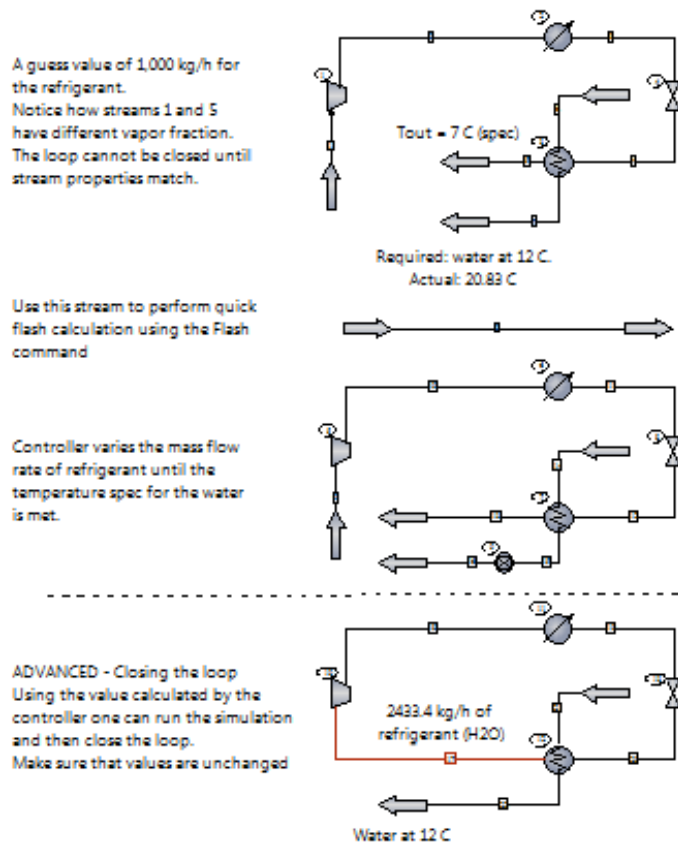
Is equal to this target: Enter the value and the units.

Note: By default, CHEMCAD's default units are used (i.e., 0 Internal unit). If any options are selected, the flowsheet global units are used for this constant.

To learn more, click the **Help** button located at the bottom left corner of the Controller dialog box.

For more on CHEMCAD's default units, see the help topic called "Neutral File Import of Component Properties." Under the Dimensional Data section, see the first line for each table of units.

Controller: Refrigeration Cycle



This example shows a simple refrigeration cycle and the use of CHEMCAD's Flash command and Controller UnitOp.

The goal is to cool 90,000 kg/h of process water from 27 °C to 12 °C. Water is used as the refrigerant.

Stream 1: Saturated steam enters the compressor at 1 kPa and is compressed to 10 kPa by specifying the outlet pressure. The compressor is adiabatic and 80% efficient based on isentropic operation.

The isolated stream is used to perform a quick flash calculation to get the temperature estimates. Specify amount, composition, pressure, and vapor fraction for the stream, then click the **Flash** button in the upper left corner of the Edit Stream dialog, to calculate temperature and enthalpy.

Guess an amount of refrigerant and specify $P = 1\text{ kPa}$ and vapor fraction = 0 to get the saturation temperature.

Note: Having saturated steam at the entrance of a compressor is risky. If the Compressor UnitOp detects any liquid in the inlet, the UnitOp ID will turn yellow and issue a warning. It is recommended to have saturated steam with a few degrees of superheat.

Stream 2: Superheated steam enters the condenser from which it emerges as a saturated liquid at 10 kPa. This is done by specifying the vapor fraction in the condenser to be 1e-005.

Stream 3: Saturated water flashes through a valve, which reduces the pressure back to 1 kPa.

Stream 4: Liquid is vaporized through the evaporator, producing saturated vapor at 1 kPa.

The water that needs to be cooled down also passes through the evaporator, thus exchanging heat with the refrigerant.

The cycle is closed when Streams 1 and 5 have the same properties.

Note: The amount of process water is known, as well as its required outlet temperature. The amount of refrigerant, however, is unknown.

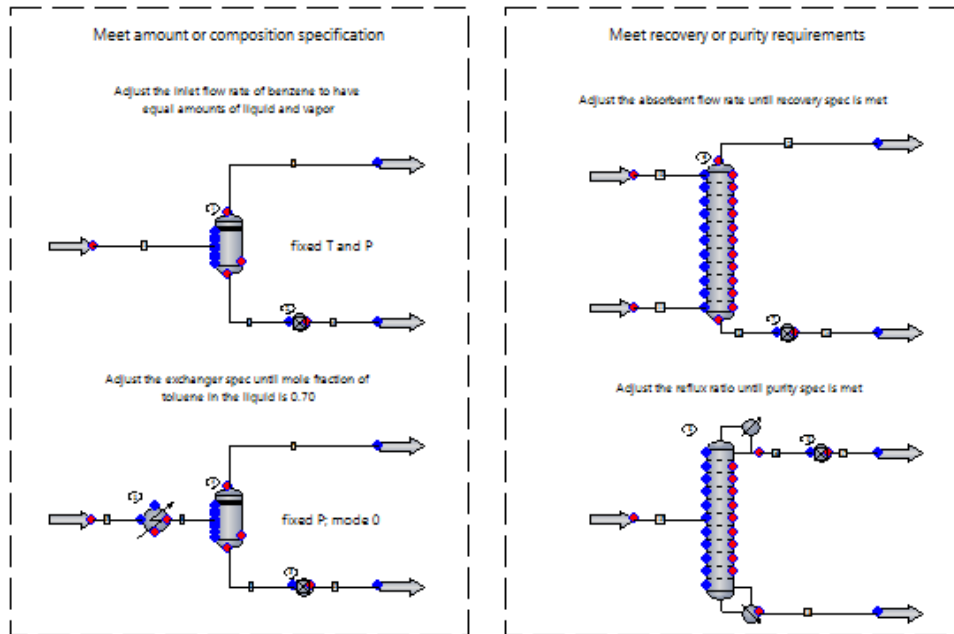
For this example, a guess of 1,000 kg/h of refrigerant was used to run the simulation. To have the same properties in streams 1 and 5, the temperature of stream 5 was specified to be 7 °C in the heat exchanger. Because the temperature of the refrigerant is specified, the temperature of the process water is allowed to vary. Here the specification is not met when a mass flow rate of 1,000 kg/h is used.

Instead of guessing the mass flow rate of refrigerant, a feed-backward controller is used. The controller "looks" at the temperature of stream 15 and manipulates the mass flow rate in stream 9 until the temperature of stream 15 is effectively 12 °C. Once the controller converges, the mass flow rate of refrigerant that results in an outlet temperature of 12 °C for the process water is replaced in the feed stream specification dialog box.

Note: this example is actually a closed cycle. However, closing the loop requires streams 9 and 13 to be very close beforehand. DO NOT attempt to draw a flowsheet from scratch with the loops closed. It is recommended to leave the flowsheet with the loop open to avoid convergence problems or convergence to a different solution.

Reference: Example modified from Abbott, M. M. & Van Ness, H. G. (1989). Schaum's Outline of Thermodynamics with Chemical Applications. New York, Mc-Graw-Hill, p. 311.

Controller: Separators



The Controller UnitOp behaves as a solver routine. The feed-backward mode, shown in this example, adjusts one variable (from an equipment or a stream) until the measured variable equals the setpoint. Scaling is allowed. The setpoint can be an algebraic calculation of two measurements.

In other words, the controller compares the measured variable to a setpoint and decides a new value for the adjusted variable until the specified condition is achieved.

The general settings tab's information flow is as follows:

Adjust this variable . . .

Until this . . .

Is equal to this target.

Adjust this variable: Specify UnitOp or stream ID, the adjusted variable and its unit, and the lower and upper bounds (do not enter if you are not sure).

Until this: Specify UnitOp or stream ID, the specification variable, and any scaling or arithmetic operation (optional).

Is equal to this target: Enter the value and the units.

Note: By default, CHEMCAD's default units are used (i.e., 0 Internal unit). If any options are selected, the flowsheet global units are used for this constant.

To learn more, click the **Help** button located at the bottom left corner of the Controller dialog box.

For more on CHEMCAD's default units, see the help topic called "Neutral File Import of Component Properties." Under the Dimensional Data section, see the first line for each table of units.